6

Optimum Design and Application of Nano-Micro-Composite Ceramic Tool and Die Materials with Improved Back Propagation Neural Network

Chonghai Xu[1,2], Jingjie Zhang[1] and Mingdong Yi[1,2]
[1]*Shandong Institute of Light Industry*
[2]*Shandong University*
PR China

1. Introduction

At present, the main method of the ceramic tool and die materials research is still the traditional 'trial-error' method which needs a large number of experiments to determine the optimum material compositions. This traditional method requires researchers to repeat experiments and to face to the complex preparation processes as well as the high cost of the experiments, and so on. Therefore, the utilization of advanced and even intelligent design technologies for ceramic material design is extremely necessary.
The computational intelligence (CI) technique, as an offshoot of artificial intelligence (AI), is a kind of heuristic algorithm including three categories: neural network, fuzzy system and evolutionary computation. Genetic algorithm (GA) and artificial neural network (ANN) are the two important computational intelligence techniques.
In recent, the two techniques especially the ANN have got successful application in the material design of ceramics and metal matrix composites, etc. For instance, some researchers used ANN to predict the functional properties of ceramic materials from compositions (Scott et al, 2007) or the bending strength and hardness of particulate reinforced Al-Si-Mg aluminum matrix composites (Altinkok & Korker, 2004) or the mechanical properties of ceramic tool (Huang et al, 2002) or the percentage of alumina in Al_2O_3/SiC ceramic cakes and the pore volume fraction (Altinkok & Korker, 2005), etc.
ANN is a kind of self-learning technology and back propagation (BP) neural network is one of the simply and commonly used network architectures. BP is based on the gradient descent method where connection weights and thresholds are modified in a direction corresponding to the negative gradient of a backward-propagated error measure (Jiang & Adeli, 2004). Although BP neural network has an advantage of high accuracy, it is often plagued by the local minimum point, low convergence or oscillation effects. In order to overcome the disadvantage of BP neural network, GA is usually used to improve the BP neural network. GA has a strong searching capability and high probability in finding the global optimum solution which is suitable for the early stage of data searching. Although these two techniques seem quite different in the number of involved individuals and the process scheme, they can provide more power of problem solving than either alone (Yen &

Lu, 2002; Yao, 1999; Gen & Cheng, 2000). Therefore, many researchers have attempted to use GA to improve BP neural network in order to achieve the complementary advantages (Sexton, 1998; Gupta & Sexton, 1999).
Some successful examples of the improved BP neural network which were optimized by GA had been reported to optimize successfully the flow stress of 304 stainless steel under cold and warm compression (Anijdan et al, 2007) or the surface roughness in end milling Inconel 718 (Ozcelik et al, 2005) or the plasma processes (Kim & Bae, 2005), etc. In literature (Zemin et al, 2010), BP neural network was used to predict punch radius based on the results of air-bending experiments of sheet metal. This prediction model was proved to be effective by experiments.
The compositions and hot pressing parameters are two important factors which can greatly affect the mechanical properties of ceramic materials. In the present study, the standard BP neural network and the improved BP neural network are used in the optimum design of both compositions and hot pressing parameters of $ZrO_2/TiB_2/Al_2O_3$ nano-micro-composite ceramic tool and die material.

2. The improved BP Neural Network

BP neural network is multi-layered forward feed neural network which is based on the error back-propagation algorithm. And the study of BP neural network can be divided into two steps which named forward-propagation process and back-propagation process, respectively. In forward-propagating process, the input is the known sample data and the information will be transmitted in turn for the hidden layer and the output layer. And the error between actual output and expected output is calculated in output layer. The back-propagation process is that the calculated error will modify each connection weight and threshold along the original way. The above two processes are iterated and repeated until the error satisfies the condition.
Fig. 1 is the structure of BP neural network. The network is multilayer which is composed of some connection neurons according to certain rules. It mainly consists of input layer, hidden layer and output layer, and each layer has independent neuron constitution. The layers are connected by the weights which can express the link degree between the neurons. And the hidden layer is composed of at least one or more layers.

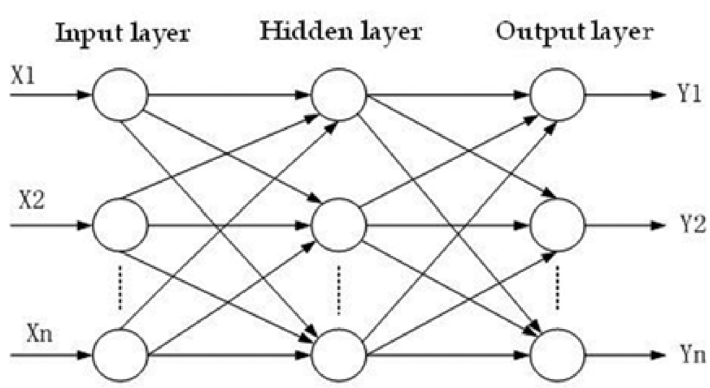


Fig. 1. The structure of BP neural network

The improved BP neural network means using GA to optimize the BP neural network. The commonly improved BP neural network mainly has three methods. One is using GA to improve the structure of BP neural network which is marked as GA-BP I; the second is using

GA to identify the initial connection weight and threshold of BP neural network which is marked as GA-BP II; while the third is using GA not only to identify the initial connection weight and threshold but also to improve the structure of BP neural network which is marked as GA-BP III. The latter two kinds of algorithms will further be discussed in the present study.

2.1 The GA-BP II algorithm

BP neural network is very sensitive to the initial vectors and different initial values may lead to completely different results. Especially in the specific calculation process, the related initial values are usually determined randomly or by experience. Once the initial value is not properly determined, it would lead to effect of oscillation or seldom convergence. Even if it is convergent, the process will be quite slow because of the too long time of training or falling into local minimum. And the best connection weights distribution can not be achieved. Used GA to optimize the connection weight and threshold of BP neural network (GA-BP II) can solve the kind of problem.

The principle of the GA-BP II algorithm is as follows: using GA to optimize the connection weights and thresholds of BP neural network from its searching space which contains all the available individuals. Then, the BP network is trained with these connection weights and thresholds so that the error between BP actual output and target output could be reduced.

2.2 The algorithm of GA-BP III

Most of the research literatures focused on the utilization of various improved GA to optimize the connection weight and threshold ignoring the importance of the structure of BP neural network and its close relationship between the structure and the connection weight. In the present study, an improved algorithm of BP neural network with GA (GA-BP III) is used for the optimum design of nano-micro-composite ceramic tool and die materials. In this algorithm, GA is used to fully optimize BP neural network including the comprehensive optimization of the structure, the initial connection weight and the threshold.

It is reported that the structure of BP neural network could greatly affect the network processing capabilities. Redundant nodes and connections are not allowed existing in a good structure. However, the design of the structure of BP neural network had not rigorously and systematically theoretical guidance and remains largely dependent on a person's experience. Using GA to solve the optimization problem of the structure can be transformed into the process of biological evolution that can be obtained through the selection, crossover and mutation, etc.

According to the Kolmogorov theorem, for three-layer BP neural network, it can achieve any given mapping. When the number of the hidden layer neurons is enough, it can use any degree of accuracy to approximate any non-linear mapping. The neurons in the input layer and output layer are determined on the specific problem; only the number of neurons in the hidden layer is variable. Thus, how to determine the number of the hidden layer neurons has become a very important issue which is the optimum object of the structure of BP neural network. If the number of neurons in the hidden layer is too little, the network may not be trained satisfyingly with the results, or the network is not robust enough with the poor fault-tolerance. If too many, they will make learning time too long and the error is not necessarily the smallest. So there exist an optimal number of the hidden layer neurons.

It is assumed that the BP neural network is hierarchically fully connected and only the neurons of two adjacent layers are possible to be connected and must be connected. If the

input and output vector values are in the real number space and there are no effects between the connected two neurons, the weight of the two connected neurons will be zero. Under the known condition of the input and output neurons, the number of the neurons in the hidden layer could only correspond to the number of the connection weight.
Thus, the principle of the GA-BP III algorithm is as following: Before the optimization, GA is used to optimize the number of connection weight, the best connection weight and threshold for BP neural network from its searching space which contains all the available individuals. After that, a global optimum solution can be achieved. Then the last generation of individuals is decoded and the corresponding structure of BP neural network, initial connection weights and thresholds can be achieved. With these values work as the structure and the initial value, samples are then trained to obtain the precise optimization. The optimum structure of BP neural network and these connection weights and thresholds could reduce the error between the output of BP neural network and the target output. Therefore, the results became more accurate.

2.2.1 Encoding

For the BP neural network with *n-d-m* three-layer where *n* is the number of neurons of the input layer, *d* is the number of neurons of the hidden layer and *m* is the number of neurons of the output layer, the floating-point type number is used for the connection weight and threshold to be encoded. Link the encoding which is encoded by the order of first connection weights then thresholds to a long string. The length of the string *L* is:

$$L=n\times d+d+d\times m+m \tag{1}$$

The scope of *d* can be ascertained by the empirical formula of the hidden layer neurons (Zhu & Shi, 2006) given below:

$$d=\sqrt{n+m}+\alpha \tag{2}$$

Where *n* and *m* can be determined based on the actual problem, α is a constant in the range of 1 to 10. Thus, once the length of the string *L* is determined, the number of hidden layer neurons and then the network structure of BP neural network can be determined. The individual value after decoding is the corresponding connection weight and threshold.

2.2.2 Determination of the fitness function

The relationship between the input and output of the network is available as following (Gu et al, 2006):

$$Y_k=\sum_{j=1}^{d}V_{jk}\cdot f\left[\sum_{i=1}^{n}W_{ij}\cdot X_i+\theta_j\right]+r_k \tag{3}$$

where f is the transfer function between layers, X_i is the actual input of the neuron i of the input layer, W_{ij} is the connection weight from the neuron i of the input layer to the neuron j of the hidden layer, θ_j is the threshold of the neuron j of the hidden layer, V_{jk} is the connection weight from the neuron j of the hidden layer to the neuron k of the output layer, r_k is the threshold of the neuron k of the output layer, and Y_k is the actual output of the neuron *k* of the output layer. According to the error between the actual output and the target output, a least-squares error function *E* can be defined as (Gu et al, 2006):

$$E(W,V,\theta,r)=\frac{1}{2p}\sum_{q=1}^{p}\sum_{i=1}^{m}(T_i^q-Y_i^q)^2 \tag{4}$$

Where *p* is the total number of the training samples, T_i^q and Y_i^q is the target output and the actual output of the neuron *i* of the input layer, respectively when the q^{th} training sample trains.
In order to integrate GA and BP, the fitness function of GA is selected as following (Gu et al, 2006):

$$f(W,V,\theta,r)=\frac{1}{E(W,V,\theta,r)+1} \tag{5}$$

In this way, once the outputs are available through the BP computation, the relating outputs are transferred to the fitness function for comparing and determining the final value. While the fitness values are being updated from generation to generation, a new generation of the population will be produced and do the same evaluation. When fitness of the population reaches the maximum, the output error of the network will become the minimum. This process will continue until the end of predetermined generation.

3. Experimental

$ZrO_2/TiB_2/Al_2O_3$ nano-micro-composite ceramic tool and die material is a typical three phase composite material in which zirconia is the matrix reinforced with titanium diboride and alumina. High purity nanometer sized ZrO_2 and micrometer sized TiB_2 and Al_2O_3 powders were used as the starting materials with average sizes of 39nm, 1.5μm and 1.0μm, respectively. According to the required volume fraction, the raw material powders were blended. The mixtures were subsequently homogenized with absolute alcohol media and Polyethylene Glycol (PEG) in a ball mill for 48h. After milling the slurry was dried in vacuum and screened.
In the experiment of compositions optimization, the samples were then formed by vacuum hot pressing (HP) technique under the hot pressing temperature of 1445°C, pressure of 30MPa and time duration of 60min. Sintered bodies were cut with a diamond wheel into samples of 3mm×4mm×30mm. The flexural strength was measured in an electronic universal testing machine (model INSTRON-5569) by means of the three-point bending method with a span of 20mm and a loading rate of 0.5mm/min. The Vickers hardness was tested by the testing machine (model Hv-120) with a load of 196N and a holding time of 15s. The fracture toughness was determined by the indentation method. The experimental data for the compositions optimization are listed in Table 1.
In the optimization process of hot pressing parameters, the pressure was kept as 35MPa limited by the hot pressing equipment. The sintering temperature was initially selected from 1420 to 1480°C and the holding time was initially selected in the range of 20-80min. All the selected hot pressing parameters are shown in Table 2. According to the processing technologies mentioned above, the materials were prepared and the mechanical properties were tested.

Number	V_{ZrO2} (%)	V_{TiB2} (%)	V_{Al2O3} (%)	Hardness (GPa)	Flexural strength (MPa)	Fracture toughness (MPa·m$^{1/2}$)
1	90	5	5	10.03	619	9.76
2	85	5	10	10.20	501	10.59
3	80	5	15	10.36	509	9.95
4	85	10	5	10.37	617	10.51
5	80	10	10	10.71	612	11.37
6	75	10	15	10.19	565	12.20
7	80	15	5	9.82	513	7.86
8	75	15	10	10.22	524	7.91
9	70	15	15	10.14	520	8.11

Table 1. The compositions and mechanical properties of $ZrO_2/TiB_2/Al_2O_3$ ceramic material

Number	Sintering temperature (°C)	Holding time (min)	Hardness (GPa)	Flexural strength (MPa)	Fracture toughness (MPa·m$^{1/2}$)
1	1430	60	13.59	1055	10.57
2	1440	60	13.78	1010	10.26
3	1450	60	13.48	878	9.54
4	1460	60	13.15	914	9.74
5	1470	60	13.26	835	9.27
6	1450	20	13.23	569	8.68
7	1450	40	12.93	671	9.91
8	1450	80	13.69	785	9.49

Table 2. The hot pressing parameters and mechanical properties of $ZrO_2/TiB_2/Al_2O_3$ ceramic material

4. The compositions optimization

4.1 The compositions optimization based on the standard BP algorithm

The BP neural network can achieve the nonlinear relationship between the compositions and the mechanical properties. If there are sufficient training data, proper change of the structure of the BP neural network which includes the number of neurons in input layer, hidden layer and output layer, and the number of the hidden layer, the BP neural network model of the optimal compositions can be established. Material compositions can then be optimized through the complex non-linear relationship between the compositions of the materials preparation and the mechanical properties. In this paper, the training sample data of standard BP neural network are the experimental data of the compositions optimization (Table 1).

The hardness, flexural strength and fracture toughness are the main mechanical properties of ceramic tool and die materials. When the processing techniques are determined, the mechanical properties of ceramic tool and die material are mainly decided by the compositions. Therefore, the inputs of the BP neural network model are the contents of each composition and the outputs are the three mechanical properties of the given materials. Therefore the model has three input neurons and three output neurons. The sigmoid-type function is adopted for the input layer to the hidden layer as the transfer function and linear-type function is adopted for the hidden layer to the output layer. And the simulated data are listed in Table 3.

Number	V_{ZrO2} (%)	V_{TiB2} (%)	V_{Al2O3} (%)	Number	V_{ZrO2} (%)	V_{TiB2} (%)	V_{Al2O3} (%)
1	85	6	9	12	80	14	6
2	85	7	8	13	75	11	14
3	85	8	7	14	75	12	13
4	85	9	6	15	75	13	12
5	80	6	14	16	75	14	11
6	80	7	13	17	60	10	30
7	80	8	12	18	60	15	25
8	80	9	11	19	60	20	20
9	80	11	9	20	60	25	15
10	80	12	8	21	60	30	10
11	80	13	7				

Table 3. The simulated data in compositions optimization

According to the theory of the BP neural network, the computing process is programmed with neural network toolbox in MATLAB. Training function is using ‘trainlm’ function and network performance parameters are using MSE function which is the mean square error between the expected output value and the actual output value to measure the network performance. The training parameters are set as following:
net.trainparam.show=10
net.train.param.goal=0.001
net.trainParam.epochs=100
net.trainParam.lr=0.01
Other parameters are set by default.

Through the calculation of the error between the actual output value and the expected output value, and according to the BP neural network model, the number of hidden layer neurons is initially chosen as 6. So, the final structure of standard BP neural network is 3×6×3. Based on this BP model, the compositions are optimized and the mechanical properties are then predicted. The predicted mechanical properties are listed in Table 4. After 62 times of iterations, the training curve of BP neural network is converged to the specified accuracy of 0.001 (Fig. 2). And the mean square error MSE is 1.24.

According to the predicted results, the best flexural strength is 643MPa and the best hardness of the materials is 9.94GPa with the corresponding volume fractions of 85vol%ZrO_2, 8vol%TiB_2 and 7vol%Al_2O_3, and the corresponding fracture toughness is 11.14MPa·$m^{1/2}$. The highest fracture toughness is 11.76MPa·$m^{1/2}$ with the corresponding volume fractions of 75vol%ZrO_2, 14vol%TiB_2 and 11vol%Al_2O_3, but the corresponding hardness and flexural strength is low. From comprehensive consideration, it seems that the mechanical properties of $ZrO_2/TiB_2/Al_2O_3$ nano-micro-composite ceramic tool and die material with the corresponding volume fractions of 85vol%ZrO_2, 8vol%TiB_2 and 7vol%Al_2O_3 is the best. So, this composition is the optimum composition in prediction.

Number	V_{ZrO2} (%)	V_{TiB2} (%)	V_{Al2O3} (%)	Hardness (GPa)	Flexural strength (MPa)	Fracture toughness (MPa·$m^{1/2}$)
1	85	6	9	9.22	546	10.91
2	85	7	8	9.06	611	11.05
3	85	8	7	9.94	643	11.14
4	85	9	6	9.89	643	10.38
5	80	6	14	9.89	506	11.27
6	80	7	13	9.88	510	11.11
7	80	8	12	9.15	543	11.11
8	80	9	11	9.87	594	9.33
9	80	11	9	9.89	594	7.36
10	80	12	8	9.00	565	6.87
11	80	13	7	9.72	547	7.24
12	80	14	6	9.75	530	11.54
13	75	11	14	9.04	568	9.68
14	75	12	13	9.06	542	8.39
15	75	13	12	9.88	528	7.95
16	75	14	11	9.28	525	11.76
17	60	10	30	9.24	451	5.91
18	60	15	25	9.81	504	6.28
19	60	20	20	9.11	576	9.77
20	60	25	15	9.12	483	10.97
21	60	30	10	9.46	454	11.05

Table 4. The predicted results of standard BP algorithm in compositions optimization

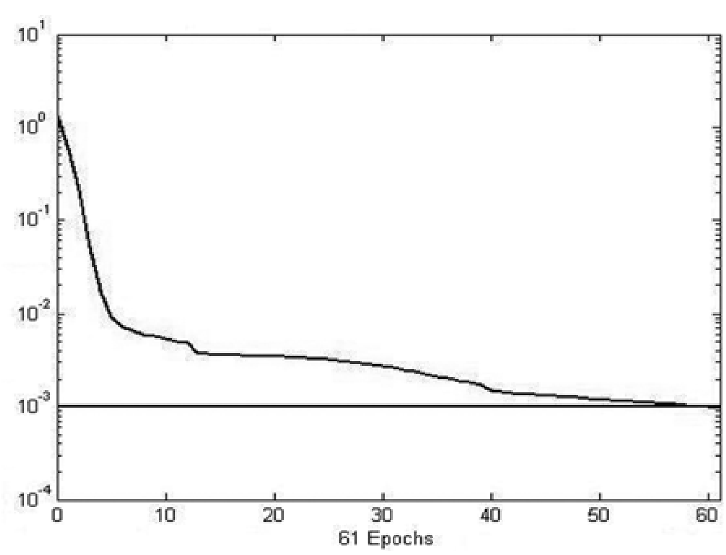


Fig. 2. The training curve of BP neural network of standard BP algorithm

4.2 The compositions optimization based on GA-BP II algorithm

According to the formerly established BP model in which the number of the neurons of hidden layer is 6 and the structure of the BP model is 3×6×3, GA-BP II algorithm is used to optimize the compositions and the predicted mechanical properties are listed in Table 5.

Number	V_{ZrO2} (%)	V_{TiB2} (%)	V_{Al2O3} (%)	Hardness (GPa)	Flexural strength (MPa)	Fracture toughness (MPa·m$^{1/2}$)
1	85	6	9	10.29	563	10.49
2	85	7	8	10.36	625	10.16
3	85	8	7	10.43	645	10.07
4	85	9	6	10.36	636	10.25
5	80	6	14	10.35	496	10.88
6	80	7	13	10.38	505	11.72
7	80	8	12	10.29	558	11.73
8	80	9	11	10.23	599	11.51
9	80	11	9	10.24	617	11.10
10	80	12	8	10.22	614	10.53
11	80	13	7	10.25	585	9.54
12	80	14	6	10.10	541	8.49
13	75	11	14	10.25	595	11.85
14	75	12	13	10.26	590	11.14
15	75	13	12	10.26	565	9.87
16	75	14	11	10.25	538	8.61
17	60	10	30	10.12	511	9.94
18	60	15	25	9.92	458	10.49
19	60	20	20	9.97	517	10.16
20	60	25	15	9.63	516	10.07
21	60	30	10	9.12	462	10.25

Table 5. The predicted results of GA-BP II algorithm in compositions optimization

After about 100 generations of searching, the fitness and square error have been stabilized respectively as shown in Fig.3. After 12 times of iterations, the training curve of BP neural network of GA-BP II algorithm is converged to the specified precision of 0.001 which is shown in Fig.4. The mean square error MSE is 1.05 and the elapsed-time is 144.20s.

According to the predicted results in Table 5, the maximum flexural strength and hardness of the materials is 645MPa and 10.43GPa,respectively, when the volume fractions of ZrO_2, TiB_2 and Al_2O_3 is 85vol%, 8vol% and 7vol%respectively while the fracture toughness is 10.07MPa·m$^{1/2}$ which is only the better one. The maximum fracture toughness of the material is 11.85MPa·m$^{1/2}$ with the corresponding volume fractions of 70vol%ZrO_2, 11vol%TiB_2 and 14vol%Al_2O_3, while the corresponding flexural strength and hardness is only 595MPa and 10.25GPa, respectively. Compared with the two compositions, the mechanical properties of the material with the volume fractions of 85vol%ZrO_2, 8vol%TiB_2 and 7vol%Al_2O_3 is the better.

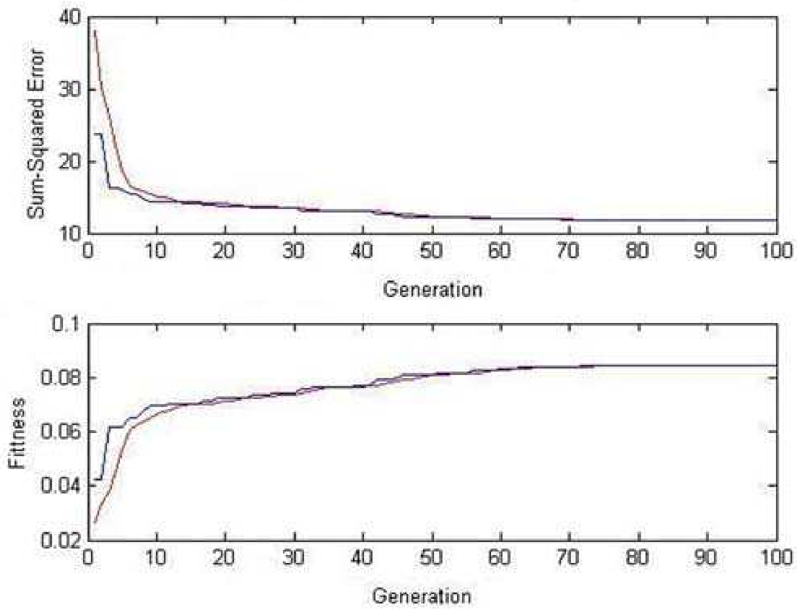


Fig. 3. The curve of square error and fitness of GA-BP II in compositions optimization

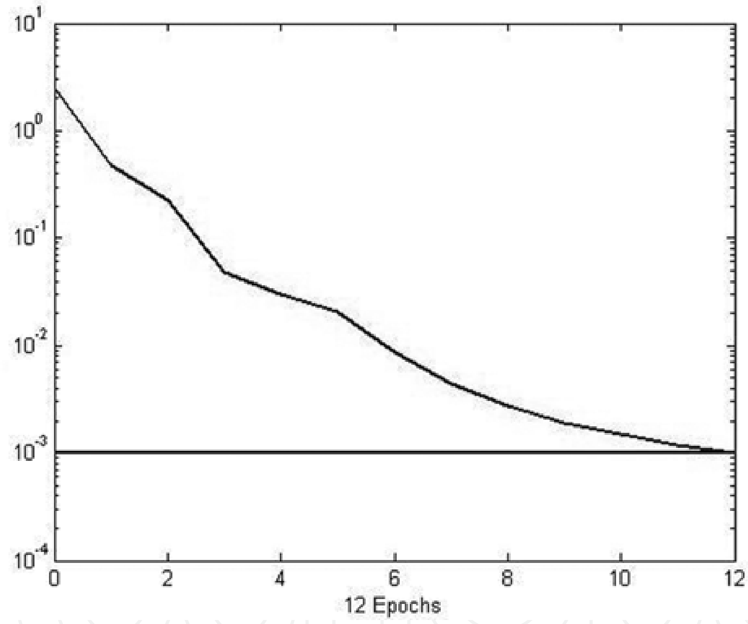


Fig. 4. The training curve of BP neural network of GA-BP II algorithm in compositions optimization

4.3 The compositions optimization based on GA-BP III algorithm

According to the compositions optimization, the input layer neuron number is 3, the output layer neuron number is 3, and the number of hidden layer neurons is set to d. According to GA-BP III algorithm, the string length L can be determined as $L=3+7d$. In accordance with the empirical formula (Eq. 2) which can determine the range of hidden layer neurons, the range of d is 4-13. According to the principle of GA-BP III algorithm, the corresponding computing process is programmed and run with MATLAB 7.0 software. The corresponding parameters are set as following: the initial population number N=30, the cross probability

P_c=0.8, the mutation probability P_m=0.1 and the error e=0.001. When the error reaches the intended target, the training process of BP neural network is then stopped.

In the process of GA optimization, with the increase of the evolution of generation, the fitness and square error are becoming convergent and finally achieve the best value. At this stage, the corresponding connection weights and thresholds of the BP neural network become the optimum. Their individuals are decoded as follows: -0.33, 1.00, 0.00, -0.64, -0.09, 0.18, -0.61, -0.38, 0.13, -0.27, -0.27, 0.91, -0.55, 0.72, 0.57, 0.33, -0.48, 0.36, -0.51, -0.19, -0.19, -0.05, 0.13, -0.32, -0.52, 0.24, -0.78, 0.29, 0.39, 0.13, -0.46, 0.00, 0.00, 0.47, 1.00, -0.32, -0.59, 0.36, -0.07, -0.40, -0.34, -0.28, -0.22, -1.00, -0.28, -0.61, 0.19, 0.49, -0.82, 0.00, 0.10, 0.52, 0.63, -0.48, 0.96, -0.89, 0.23, 0.11, -0.59. Based on the above 59 parameters and $L=3+7d$, the number of hidden layer neurons is ascertained as 8. Therefore the structure of BP neural network is 3×8×3 and the last 11 parameters are the threshold values. Some connection weights in the list above are found to be 0.00 which indicate that the connection between the two neighboring neurons is invalid.

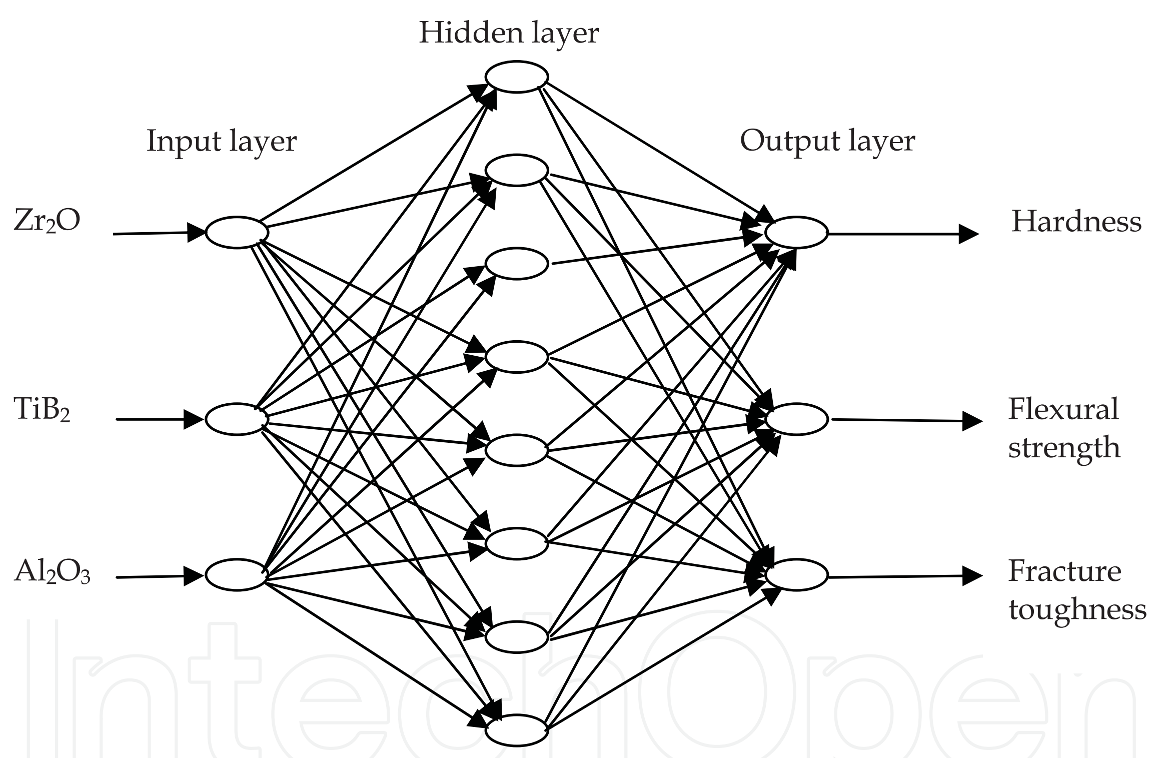


Fig. 5. The structure of BP neural network of GA-BP III algorithm in compositions optimization

The concrete structure of BP neural network is the improved BP neural network optimized by GA which is shown in Fig.5. It can be seen that the first neuron of input layer and the third neuron of hidden layer is no connection. The third neuron of hidden layer and the second and the third neurons of output layer are also connectionless. The data within the range of the experimental results are selected as the data for prediction in order to get the optimum compositions corresponding to the best mechanical properties.

After about 100 generations of searching, the fitness and the square error have been stabilized respectively as shown in Fig.6. The curve of BP training target is shown in Fig.7. It indicates that the BP neural network has 8 iterations convergence to the specified accuracy. The elapsed-time is 129.939s and MSE is 0.1491.

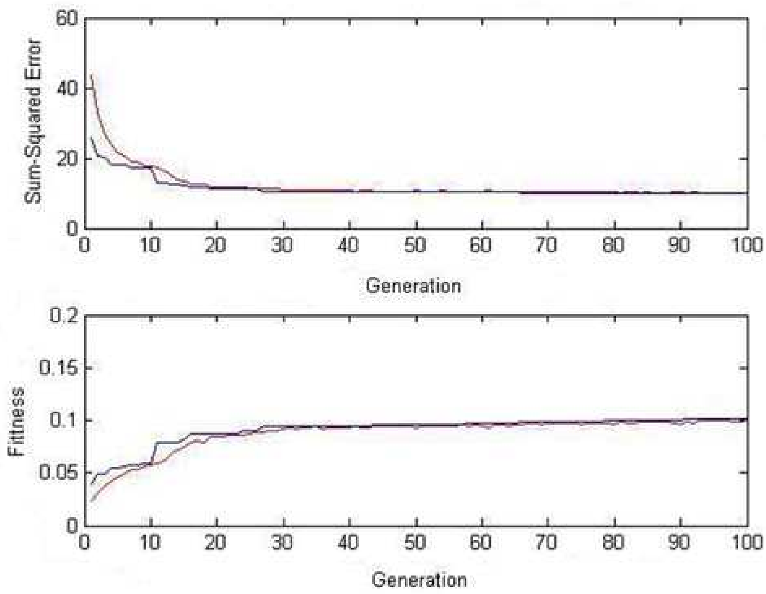


Fig. 6. The curve of square error and fitness of GA-BP III algorithm in compositions optimization

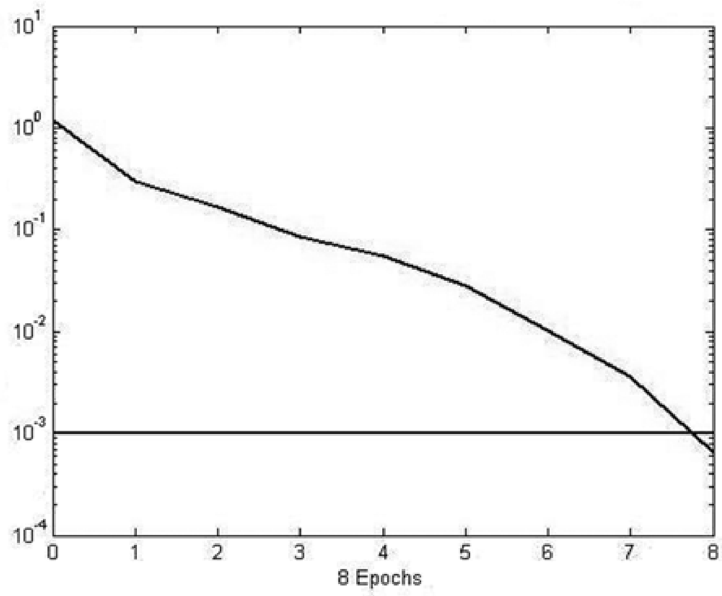


Fig. 7. The training curve of BP neural network of GA-BP III algorithm in compositions optimization

The predicted results of GA-BP III algorithm are given in Table 6. It indicates that the highest flexural strength is 685MPa and the highest hardness is 10.74GPa with the corresponding volume fractions of 85vol%ZrO_2, 8vol%TiB_2 and 7vol%Al_2O_3. The fracture toughness with the same compositions is 10.38MPa.m$^{1/2}$ which is slightly less than the best value 11.72 MPa.m$^{1/2}$ when the volume fraction of ZrO_2, TiB_2 and Al_2O_3 is 80%, 9% and 11%, respectively. While the flexural strength and hardness with the latter compositions is only 568 MPa and 10.72GPa, respectively. It suggests that comprehensive good mechanical properties of the namo-micro-composite ceramic tool and die material $ZrO_2/TiB_2/Al_2O_3$ can be achieved when the volume fraction of ZrO_2, TiB_2 and Al_2O_3 is 85%, 8% and 7%, respectively.

Number	V_{ZrO2} (%)	V_{TiB2} (%)	V_{Al2O3} (%)	Hardness (GPa)	Flexural strength (MPa)	Fracture toughness (MPa ·m$^{1/2}$)
1	85	6	9	10.41	581	10.33
2	85	7	8	10.62	652	10.24
3	85	8	7	10.74	685	10.38
4	85	9	6	10.68	674	10.50
5	80	6	14	10.58	525	10.73
6	80	7	13	10.69	537	11.28
7	80	8	12	10.72	547	11.63
8	80	9	11	10.72	568	11.72
9	80	11	9	10.66	662	10.66
10	80	12	8	10.47	657	9.94
11	80	13	7	10.10	590	9.15
12	80	14	6	9.89	538	8.39
13	75	11	14	10.33	539	11.41
14	75	12	13	10.42	519	10.50
15	75	13	12	10.46	510	9.69
16	75	14	11	10.43	517	8.90
17	60	10	30	9.74	567	7.33
18	60	15	25	9.75	567	7.27
19	60	20	20	9.76	567	7.24
20	60	25	15	9.06	407	7.05
21	60	30	10	9.76	506	5.75

Table 6. The predicted results of GA-BP III algorithm in compositions optimization

4.4 Results and discussion

According to the above predicted results of three algorithms (BP/GA-BP II/GA-BP III) and the analysis, 85%ZrO_2, 8vol%TiB_2 and 7vol%Al_2O_3 are chosen as the optimum compositions since material with the ingredients will have the best flexural strength, the best hardness and the better fracture toughness. Then, $ZrO_2/TiB_2/Al_2O_3$ nano-micro-composite ceramic tool and die material with the above optimum compositions is prepared with the vacuum hot pressing techniques described in section 3. Compared with the above two algorithms, the GA-BP III algorithm has less iteration number, shorter elapsed-time and smaller MSE.

Both the experimental data and the predicted data of these kinds of methods mentioned above are all listed in Table 7 as well as the relative errors between the predicted and experimental data. It can be seen that the two kinds of the improved algorithms of both GA-BP II algorithm and GA-BP III algorithm all have higher prediction accuracy than the standard BP algorithm. However, the GA-BP III algorithm has the least relative error among the three algorithms. The least relative error of the hardness, flexural strength and fracture toughness is 1.8%, 1.4% and 0.7%, respectively which is approximately 38%, 20% and 32% of that of GA-BP II algorithm and 20%, 19% and 9% of that of standard BP algorithm. The predicted data of GA-BP III algorithm better coincide with the experimental data. Therefore, it can well be used in the compositional design of ceramic tool and die materials with high accuracy of prediction and high reliability.

	Hardness (GPa)	Relative error (%)	Flexural strength (MPa)	Relative error (%)	Fracture toughness ($MPa \cdot m^{1/2}$)	Relative error (%)
Experimental	10.95	/	694	/	10.30	/
Standard BP	9.94	9.2	643	7.4	11.14	8.1
GA-BPII	10.43	4.7	645	7.1	10.07	2.2
GA-BPIII	10.74	1.8	685	1.4	10.38	0.7

Table 7. Comparison of the optimal results of three algorithms and experimental results of the ZrO_2 based ceramic tool and die material with 8vol%TiB_2 and 7vol%Al_2O_3

5. The optimization of hot pressing parameters

As is known, the mechanical properties of ceramic materials depend on the composition and microstructure of the material. So in addition to the material compositions, the hot pressing parameters are the main factors affecting the microstructure and the mechanical properties. When one of the hot pressing parameters is changed, the sample material is needed to prepare and the mechanical properties have to be tested. If it is necessary, microstructural and phase analysis will even be needed to do. This will result in the disadvantages of high cost and long time-consuming, etc. In this section, the standard BP neural network and the improved BP neural network GA-BP II and GA-BP III are used to optimize the hot pressing parameters of $ZrO_2/TiB_2/Al_2O_3$ namo-micro-composite ceramic tool and die materials. And based on the optimum results, the materials are then prepared and mechanical properties are tested in order to validate the optimization algorithms.

5.1 The optimization of hot pressing parameters based on the standard BP algorithm

BP neural network can also be used to achieve the nonlinear mapping relationship between the hot pressing parameters and the mechanical properties of the ceramic tool and die material.

The training sample data of BP neural network are the experimental data (Table 2). The input is the hot pressing parameters, including the sintering temperature and holding time. And the output is the main mechanical properties, including hardness, flexural strength and fracture toughness. Simulated data are selected from all the data in range of the sintering temperature and holding time, which are listed in Table 8.

Based on the actual optimal problem, there are two inputs and three outputs of the BP neural network model. Therefore, the BP model is then established, which has two input neurons and three output neurons. The transfer function is sigmoid-type and linear-type in the hidden layer and output layer, respectively.

Number	Sintering temperature (ºC)	Holding time (min)	Number	Sintering temperature (ºC)	Holding time (min)
1	1420	20	11	1460	20
2	1420	40	12	1460	40
3	1420	60	13	1460	80
4	1420	80	14	1470	20
5	1430	20	15	1470	40
6	1430	40	16	1470	80
7	1430	80	17	1480	20
8	1440	20	18	1480	40
9	1440	60	19	1480	60
10	1440	80	20	1480	80

Table 8. The simulated data in the optimization of hot pressing parameters

According to the theory of the BP neural network, the computing process is programmed with neural network toolbox in MATLAB. Training function is using 'trainlm' function and network performance parameters is using MSE function. The training parameters are set as the same as that in the compositions optimization. And other parameters are set by default.

Number	Sintering temperature (ºC)	Holding time (min)	Hardness (GPa)	Flexural strength (MPa)	Fracture toughness (MPa·m$^{1/2}$)
1	1420	20	13.55	726	10.26
2	1420	40	13.58	751	10.03
3	1420	60	12.94	1151	12.15
4	1420	80	12.55	1104	11.10
5	1430	20	13.55	722	10.23
6	1430	40	13.49	764	10.47
7	1430	80	12.70	1085	11.97
8	1440	20	13.45	673	9.76
9	1440	60	13.78	1001	10.27
10	1440	80	13.24	984	11.23
11	1460	20	13.19	543	8.52
12	1460	40	12.72	700	10.13
13	1460	80	13.80	722	8.54
14	1470	20	13.29	521	8.21
15	1470	40	12.80	700	9.91
16	1470	80	14.43	614	6.37
17	1480	20	14.00	371	6.04
18	1480	40	13.20	635	8.73
19	1480	60	13.16	816	9.40
20	1480	80	14.53	618	5.90

Table 9. The predicted results of standard BP algorithm in the optimization of hot pressing parameters

According to the BP neural network model, the number of hidden neurons is initially chosen as 6, so the neural network structure is 2×6×3. Based on this BP model, the hot pressing parameters are optimized and the mechanical properties are obtained by prediction. Because of the differences of the initial data, the BP neural network is easy to be shocked, especially in the optimization parameters. Under such circumstances, four times of the separate BP neural network prediction and simulation is carried out, but the result of each MSE is not the same. The MSE = 6.45 is selected which is nearly the average value in the four times, and the predicted results are listed in Table 9. After 40 times of iterations, the training curve of BP neural network is converged to the specified precision of 0.001.
According to the predicted results, the highest flexural strength and fracture toughness of the materials is 1151MPa and 12.15 MPa·$m^{1/2}$, respectively when the sintering temperature is 1420°C and the holding time is 60min, while the hardness is just 12.94GPa. The highest hardness of the material is 14.53GPa which corresponds to the sintering temperature of 1480°C and the holding time of 80min. In this case, the flexural strength of the material is 618MPa and the fracture toughness is 5.90 MPa·$m^{1/2}$. The hardness of the material which is prepared with these hot pressing parameters reaches the highest, but both flexural strength and fracture toughness are relative low. Compared with the mechanical properties of the ceramic tool and die materials prepared with different hot pressing parameters, it seems that the ceramic tool and die material which is fabricated with sintering temperature of 1420°C and holding time of 60min has better comprehensive mechanical properties. Therefore, these hot pressing parameters are the optimum hot pressing parameters for the fabrication of $ZrO_2/TiB_2/Al_2O_3$ namo-micro-composite ceramic tool and die material.

5.2 The optimization of hot pressing parameters based on GA-BP II algorithm

According to the formerly established BP model where the number of the neurons of hidden layer is 6 and the structure of the BP model is 2×6×3, the GA-BP II algorithm is then utilized to optimize the hot pressing parameters. The mechanical properties are obtained and given in Table 10. After 40 times of iterations, the training curve of BP neural network of GA-BP II algorithm is converged to the specified precision of 0.001. The mean square error MSE is 4.27.
After analyzing the predicted results, the material is prepared with the sintering temperature of 1420°C and the holding time of 60min. It has the best flexural strength and the best fracture toughness which is 1052MPa and 10.59 MPa·$m^{1/2}$, respectively. Under the same hot pressing parameters, however, the hardness of the material is 13.36GPa which is slightly lower. The highest hardness of the material amounts to be 14.28GPa where the corresponding sintering temperature is 1420°C and the holding time is 80min, while the flexural strength is 1051MPa and the fracture toughness is 10.40 MPa·$m^{1/2}$. Compared with the mechanical properties of ceramic tool and die material which is prepared in different hot pressing parameters, it suggests that the comprehensive good mechanical properties of $ZrO_2/TiB_2/Al_2O_3$ namo-micro-composite ceramic tool and die material can be achieved when the sintering temperature is 1420°C and the holding time is 60min.

5.3 The optimization of hot pressing parameters based on GA-BP III algorithm

According to the actual problem, the input layer neuron number is 2, the output layer neuron number is 3, and the number of hidden layer neurons is set to d. According to GA-BP III algorithm, the string length L can be determined as $L=3+6d$. In accordance with the

Number	Sintering temperature (ºC)	Holding time (min)	Hardness (GPa)	Flexural strength (MPa)	Fracture toughness (MPa·m $^{1/2}$)
1	1420	20	14.25	1042	10.39
2	1420	40	14.27	1035	10.51
3	1420	60	13.36	1052	10.59
4	1420	80	14.28	1051	10.40
5	1430	20	13.37	776	9.91
6	1430	40	14.17	1037	10.31
7	1430	80	13.26	1050	10.30
8	1440	20	12.82	624	9.92
9	1440	60	13.78	1010	10.26
10	1440	80	13.31	1035	10.54
11	1460	20	12.83	857	8.42
12	1460	40	12.42	870	9.77
13	1460	80	13.86	597	8.21
14	1470	20	12.15	1006	8.94
15	1470	40	12.29	1005	8.92
16	1470	80	13.29	985	8.87
17	1480	20	12.23	1000	8.87
18	1480	40	13.62	826	7.63
19	1480	60	14.05	704	7.53
20	1480	80	13.25	831	9.11

Table 10. The predicted results of GA-BP II algorithm in the optimization of hot pressing parameters

empirical formula (Eq. 2) which can determine the range of hidden layer neurons, the range of d is 3-12. According to the principle of GA-BP III algorithm, the computing process are programmed and run with MATLAB 7.0 software. The corresponding parameters are set as following: the initial population number N=30, the cross probability P_c=0.8, the mutation probability P_m=0.1 and the error e=0.001. When the error reaches the intended target, the training parameters of BP neural network is then stopped.

The individuals of the connection weight and thresholds are decoded as follows: 0.32, -0.14, 0.36, -0.29, 0.24, 0.16, 0.24, -0.88, -0.24, 0.16, -0.16, 0.60, 0.44, -0.69, -0.40, 0.03, 0.26, 1, 0.39, -0.29, 0.21, -0.49, 0.00, 1, -0.20, -1, -1, -0.68, 0.00, 0.00, 0.35, 0.02, 0.32, -0.27, 1, 0.09, -0.13, -0.23, 0.15.

Based on the above 39 parameters and $L=3+6d$, the number of hidden layer neurons is ascertained as 6. Therefore, the structure of BP neural network is 2×6×3 and the last 9 parameters are the threshold values. The structure is shown in Fig.8 which is the optimal BP neural network of GA-BP III algorithm. It can be seen that the second neuron of input layer and the fifth neuron of hidden layer is no connection. The sixth neuron of hidden layer and the second and third neurons of output layer are also connectionless. After about 100 generations of searching, the fitness and the square error have been stabilized respectively as shown in Fig. 9. The curve of BP training target is shown in Fig. 10. It is shown that the BP neural network has 45 iterations convergence to the specified accuracy. The elapsed-time is 155.584s and the MSE is 0.1643.

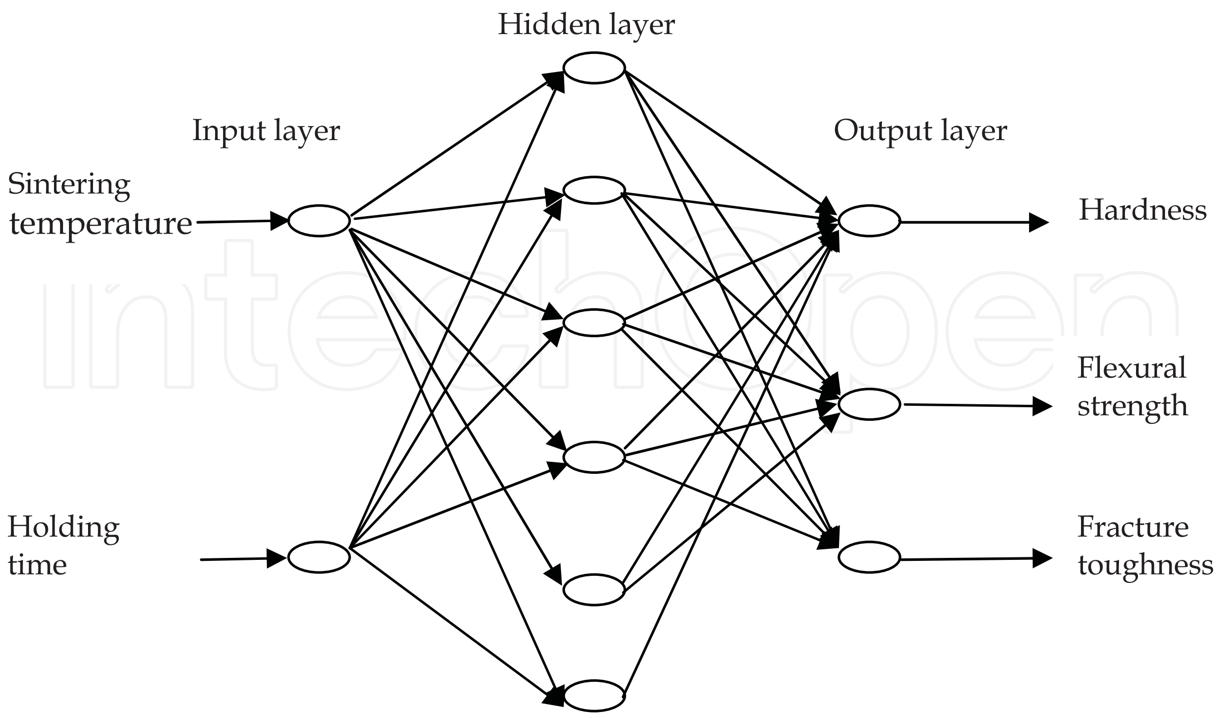


Fig. 8. The structure of BP neural network for GA-BP III algorithm simulation in the optimization of hot pressing parameters

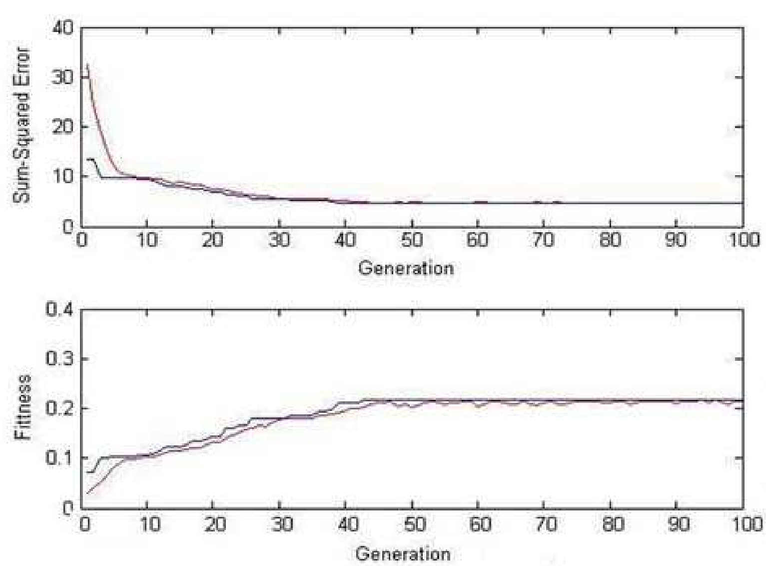


Fig. 9. The curve of square error and fitness of GA-BP III algorithm in the optimization of hot pressing parameters

The predicted results of GA-BP III algorithm are given in Table 11. It can be seen that the optimum flexural strength and the optimum fracture toughness is 1010MPa and 10.40 MPa·m$^{1/2}$ respectively when the material is prepared with the sintering temperature of 1420°C and the holding time of 60min. The hardness of the material fabricated in these hot pressing parameters is 13.43GPa. The optimum hardness is 14.14GPa which is corresponding to the sintering temperature of 1420°C and the holding time of 80min, while

Number	Sintering temperature (ºC)	Holding time (min)	Hardness (GPa)	Flexural strength (MPa)	Fracture toughness (MPa ·m$^{1/2}$)
1	1420	20	13.72	1002	10.91
2	1420	40	13.70	1004	10.38
3	1420	60	13.43	1010	10.40
4	1420	80	14.14	804	9.55
5	1430	20	13.71	996	10.34
6	1430	40	13.71	1005	10.38
7	1430	80	14.02	858	8.06
8	1440	20	13.62	818	9.80
9	1440	60	13.78	1005	10.27
10	1440	80	14.06	897	8.20
11	1460	20	12.08	768	9.82
12	1460	40	11.95	827	9.31
13	1460	80	13.52	493	8.56
14	1470	20	11.69	850	9.96
15	1470	40	12.30	885	9.67
16	1470	80	13.63	427	8.38
17	1480	20	11.70	857	9.96
18	1480	40	12.96	909	9.19
19	1480	60	13.42	715	8.46
20	1480	80	13.66	431	8.37

Table 11. The predicted results of GA-BP III algorithm in the optimization of hot pressing parameters

the flexural strength and fracture toughness is just 804MPa and 9.55MPa ·m$^{1/2}$, respectively. Both values are obviously lower than the optimum. Therefore, the optimum hot pressing parameters are that the sintering temperature is 1420°C and the holding time is 60min which is the same as that of GA-BP II algorithm.

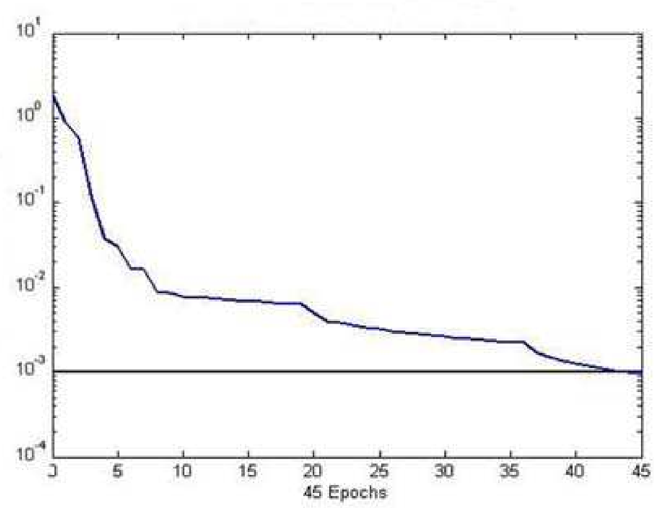


Fig. 10. The training curve of BP neural network of GA-BP III algorithm in the optimization of hot pressing parameters

5.4 Results and discussion

According to the predicted results of three algorithms, the sintering temperature of 1420°C and holding time of 60min are determined as the optimum hot pressing parameters. Then, with these optimized hot pressing parameters, $ZrO_2/TiB_2/Al_2O_3$ nano-micro composite ceramic tool and die material with the above optimum compositions is prepared by means of the vacuum hot pressing technique described in section 3 and mechanical properties are tested.

	Hardness (GPa)	Relative error (%)	Flexural strength (MPa)	Relative error (%)	Fracture toughness (MPa·m$^{1/2}$)	Relative error (%)
Experimental	13.3	/	937.0	/	10.17	/
Standard BP	12.9	2.8	1151.5	22.8	11.10	9.1
GA-BP II	13.4	0.9	1052.5	12.3	10.60	4.2
GA-BP III	13.4	0.9	1009.7	7.8	10.40	2.2

Table 12. Comparison of the optimal results of three algorithms and experimental results in the optimization of hot pressing parameters

Table 12 gives the experimental mechanical properties of the $ZrO_2/TiB_2/Al_2O_3$ nano-micro-composite ceramic tool and die material which is prepared under the optimum hot pressing parameters. The predicted results and the relative errors are both listed.

Compared with the experimental values, the least relative error of flexural strength and fracture toughness is 7.8% and 2.2% obtained by GA-BP III algorithm which is approximately 63% and 48% of that of GA-BP II algorithm and 34% and 24% of that of standard BP algorithm. The least relative error of hardness is 0.9% obtained by GA-BP III algorithm which is the same as that obtained by GA-BP II algorithm. In addition to the same relative error of hardness by GA-BP II algorithm, other relative errors of mechanical properties by GA-BP III are the least. So the predicted results of GA-BP III algorithm are the most accurate in these three algorithms. The predicted data of GA-BP III algorithm better coincide with the experimental data. Therefore, it can well be utilized for the optimum design of hot pressing parameters of ceramic tool and die materials with high accuracy of prediction and reliability.

6. Conclusion

With the utilization of GA-BP III algorithm for the compositional design of nano-micro-composite ceramic tool and die material, the iteration number could noticeably be reduced and results are more accurate. It can avoid the local minimum problem and can present more accurate and reliable results. And it also can overcome the disadvantages of both long time and slow speed of the standard BP neural network. Preparation experiments of $ZrO_2/TiB_2/Al_2O_3$ nano-micro-composite ceramic tool and die material indicate that the relative error between the experimental and predicted results of the hardness, flexural strength and fracture toughness is 1.8%, 1.4% and 0.7%, respectively by the GA-BP III algorithm which is the least relative error among three kinds of algorithms. The predicted data better coincide with the experimental data high accuracy of prediction.

The GA-BP III algorithm can also well be used in the optimization of hot pressing parameters of nano-micro-composite ceramic tool and die material. It can reduce the number of iterations. The optimization results are more precise. The GA-BP III algorithm can avoid falling into local minimum which is the shortcoming of standard BP algorithm, and can obtain more accurate and reliable optimization results. Compared with the experimental results and the predicted result of standard BP neural network, it indicates that the improved BP algorithms, especially GA-BP III algorithm are suitable for the optimization of hot pressing parameters of $ZrO_2/TiB_2/Al_2O_3$ nano-micro-composite ceramic tool and die materials.

Therefore, the GA-BP III algorithm is one of the fast, effective and reliable algorithms in the optimum design of both compositions and hot pressing parameters of nano-micro-composite ceramic tool and die materials. It suggests that it can also be effectively applied in the material design area of other ceramic composites.

7. Acknowledgement

This work was supported by Shandong Provincial Natural Science Foundation, China (Grant No. ZR2009FZ005), the Program for New Century Excellent Talents in University of China (Grant No. NCET-10-0866), the National Natural Science foundation of China (Grant No. 51075248), Shandong Provincial Natural Science Foundation for Distinguished Young Scientists, China (Grant No. JQ201014).

8. References

Altinkok N. & Korker R. N. (2004). Neural Network Approach to Prediction of Bending Strength and Hardening Behaviour of Particulate Reinforced (Al-Si-Mg) Aluminium Matrix Composites. *Materials and Design*, Vol. 25, No. 7, Oct, 2004, pp. 595-602, ISSN 0261-3069

Altinkok N. & Korker R. N. (2005). Mixture and Pore Volume Fraction in Al_2O_3/SiC Ceramic Cake Using Artificial Neural Networks. *Materials and Design*, Vol. 26, No. 4, Jun, 2005, pp. 305-311, ISSN 0261-3069

Gen M. & Cheng R. (2000). *Genetic algorithm and Engineering Optimization*, Wiley, ISBN 0-471-31531-1, New York

Gu X.Q.; Yi D.X & Liu C.H. (2006). Optimization of Topological Structure and Weight Value of Artifical Neural Network using Genetic Algorithm. *Journal of Guangdong University of Technology*, Vol. 23, No. 4, 2006, pp. 64-69, ISSN 1007-7162 (in Chinese)

Gupta J.N.D. & Sexton R.S. (1999). Comparing Back propagation with a Genetic Algorithm for Neural Network Training. *The International Journal of Management Science*. Vol. 27, Dec, 1999, pp. 679-684, ISSN 1226-0797

Huang C.Z.; Zhang L.; He L.; Sun J.; Fang B. & B. Zou. J. (2002). A Study on the Prediction of the Mechanical Properties of a Ceramic Tool Based on an Artificial Neural Network. *Journal of Materials Processing Technology*, Vol. 129, Oct, 2002, pp. 399-402, ISSN 0924-0136

Jiang X. & Adeli H. (2004). Clustering-Neural Network Models for Freeway Work Zone Capacity Estimation. *International Journal of Neural Systems*, Vol. 14, No. 3, Jun, 2004, pp. 147-163, ISSN 0129-0657

Kim B. & Bae J. (2005). Prediction of Plasma Processes Using Neural Network and Genetic Algorithm. *Solid-State Electronics*, Vol. 49, Oct, 2005, pp. 1576-1580, ISSN 0038-1101

Mousavi Anijdan S.H.; Madaah-Hosseini H.R. & Bahrami A. (2007). Flow stress Optimization for 304 Stainless Steel under Cold and Warm Compression by Artificial Neural Network and Genetic Algorithm. *Materials and Design*, Vol. 28, 2007, pp. 609-615, ISSN 0261-3069

Ozcelik B.; Oktem H. & Kurtaran H. (2005). Surface Roughness in End Milling Inconel 718 by Coupling Neural Network Model and Genetic Algorithm. *The International Journal of Advanced Manufacturing Technology*, Vol. 27, 2005, pp. 234-241, ISSN 0268-3768

Scott D.J.; Coveney P.V.; Kilner J.A.; Rossing J.C.H.; Alford N.M. & Ceram J. (2007). Prediction of the Functional Properties of Ceramic Materials from Composition Using Artificial Neural Networks. *Journal of the European Ceramic Society*, Vol. 27, Dec, 2007, pp. 4425-4435, ISSN 0955-2219

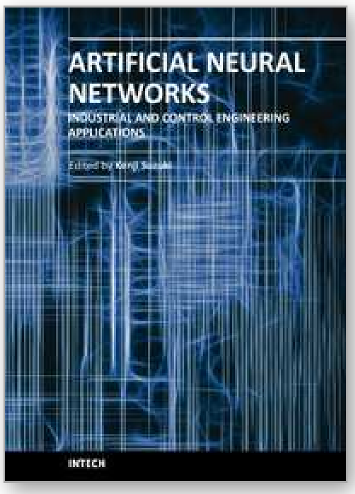
Sexton R.S.; Dorsey R.E. & Johnson J.D. (1998). Toward Global Optimization of Neural Network: A Comparison of the Genetic Algorithm and Backpropagation. *Decision Support Systems*. Vol. 22, Feb, 1998, pp. 171-185, ISSN 0167-9236

Yao X. (1999). Evolving Artificial Neural Network, *Proceedings of IEEE*, pp. 1423-1447, ISBN 0018-9219, Sep 1999, IEEE Press. Vol. 87

Yen G.& Lu H. M. (2002). Hierarchical Genetic Algorithm for Near-Optimal Feed Forward Neural Network Design. *International Journal Neural Systems*, Vol. 12, No. 1, Feb, 2002, pp. 31-43, ISSN 0129-0657

Zemin F.; Jianhua M. & Lin C. (2010). Using Genetic Algorithm-Back Propagation Neural Network Prediction and Finite-element Model Simulation to Optimize the Process of Multiple-step Incremental Air-bending Forming of Sheet Metal. *Materials and Design*, Vol. 31, Jan, 2010, pp. 267-277, ISSN 0261-3069

Zhu D.Q. & Shi H. (2006). *The Principle and Application of Artificial Neural Networks*, Science Press, ISBN 7-03-016570-5, Beijing (in Chinese)



Artificial Neural Networks - Industrial and Control Engineering Applications
Edited by Prof. Kenji Suzuki

ISBN 978-953-307-220-3
Hard cover, 478 pages
Publisher InTech
Published online 04, April, 2011
Published in print edition April, 2011

Artificial neural networks may probably be the single most successful technology in the last two decades which has been widely used in a large variety of applications. The purpose of this book is to provide recent advances of artificial neural networks in industrial and control engineering applications. The book begins with a review of applications of artificial neural networks in textile industries. Particular applications in textile industries follow. Parts continue with applications in materials science and industry such as material identification, and estimation of material property and state, food industry such as meat, electric and power industry such as batteries and power systems, mechanical engineering such as engines and machines, and control and robotic engineering such as system control and identification, fault diagnosis systems, and robot manipulation. Thus, this book will be a fundamental source of recent advances and applications of artificial neural networks in industrial and control engineering areas. The target audience includes professors and students in engineering schools, and researchers and engineers in industries.