ISSN 1027-5495. Functional Materials, 26, No.4 (2019), p. 823-828.
doi:https://doi.org/10.15407/fm26.04.823

Application of immune genetic algorithm in optimization of nanocomposite metal materials

K.Xian

Sichuan College of Architectural Technology, Sichuan, China

Received May 20, 2019

In order to study the application of immune genetic algorithm in the optimization of nano-composite metal materials, a new algorithm based on immune genetic mechanism was proposed. The problems such as precocity of genetic algorithm, low searching efficiency and inability to maintain individual diversity were avoided, and the corresponding material components were obtained. The optimization results show that the immune genetic algorithm converges in the 10th generation, and the convergence speed of the immune genetic algorithm increases by 50 %, 40 % and 37.5 %, respectively. The convergence rate of the immune genetic algorithm is faster than that of the immune algorithm, and the optimal component is obtained. The application of the fracture toughness in the optimization of nanocomposite metal materials is explored, which is of great significance for improving the efficiency of ceramic mold material design.
Keywords: immune inheritance, nanocomposite metal, optimization.

Для возможности применения иммуногенетического алгоритма в оптимизации нанокомпозитных металлических материалов предложен новый алгоритм. Игнорировались такие проблемы, как скороспелость генетического алгоритма, низкая эффективность поиска и неспособность поддерживать индивидуальное разнообразие. Получены соответствующие компоненты. Результаты оптимизации показывают, что иммуногенетический алгоритм сходится в 10-м поколении, скорость конвергенции иммуногенетического алгоритма увеличивается на 50 %, 40 % и 37,5 % соответственно. Скорость сходимости иммунного генетического алгоритма выше, чем у иммунного алгоритма. Используя полученный алгоритм, изучено применение трещиностойкости при оптимизации нанокомпозитных металлических материалов, что имеет большое значение для повышения эффективности конструирования керамического литейного материала.

Застосування імуногенетичного алгоритму в оптимізації нанокомпозитних металевих матеріалів. *K.Xian*.
Для можливості застосування імуногенетичного алгоритму в оптимізації нанокомпозитних металевих матеріалів запропонований новий алгоритм. Ігнорувалися такі проблеми, як скоростиглість генетичного алгоритму, низька ефективність пошуку і нездатність підтримувати індивідуальну різноманітністю. Отримано відповідні матеріальні компоненти. Результати оптимізації показують, що імуногенетичний алгоритм сходиться у 10-му поколінні, і швидкість конвергенції імуногенетичного алгоритму збільшується на 50 %, 40 % і 37,5 % відповідно. Швидкість збіжності імуногогенетичного алгоритму вище, ніж у імунного алгоритму. Використовуючи отриманий алгоритм, вивчено застосування тріщиностійкості при оптимізації нанокомпозитних металевих матеріалів, що має велике значення для підвищення ефективності конструювання керамічного ливарного матеріалу.

1. Introduction

At present, in the optimization design process of nanocomposites, continuous experiments are required, adjust the composition ratio of materials and preparation process, then obtain the best performance materials. Among the experimental process, considering the complexity, the high cost, the complexity of the material preparation process and the long experimental period, this method needs to combine advanced intelligent computing technology to improve the design efficiency of nanocomposites [1].

The Artificial Immune System (AIS) is an intelligent method that simulates the functions of the natural immune system. It has an evolutionary learning mechanism without teacher learning, self-organization and memory, and combines systems advantages of classifiers, neural networks and machine inference [2]. The genetic algorithm is an algorithm based on biological genetics and evolutionary mechanism proposed by Professor Holland of the United States. It draws on Darwin's theory of evolution and Mendel's genetic theory [3]. Through random selection, crossover, and mutation operations, the population evolves and converges to the individual that best fits the target.

Among the design and performance optimization of nanocomposites, Research and use of more computational intelligence technologies are composite algorithm of artificial neural networks, genetic algorithms and a combination of the two, but they all have defects, which limits their further application development. At present, there are many researches on immune algorithm and its combination with genetic algorithm. This combination algorithm can overcome the shortcomings of the two algorithms when used alone, such as premature convergence and local optimization. The immune algorithm and immune genetic algorithm are applied to the optimization design of nanocomposites, which can provide a novel computational intelligent design method of nanocomposites, further improve the efficiency of nanocomposite optimization design, and shorten the development cycle of ceramic mold materials [4].

In this paper, Ti(C,N)-based nanocomposite cermet mold materials are the object [5], combining immune algorithm with genetic algorithm to optimize nanocomposite design, the application of immune genetic algorithm in nanocomposite optimization is studied. It is important to improve the optimization design efficiency of Ti(C,N)-based nanocomposite metal nano-die materials.

2. Construction of mathematical model for optimization design of nanocomposite metal materials based on immune genetic algorithm

2.1 Mathematical model between fracture toughness and composition of nanocomposite cermet mold materials

The ceramic mold materials studied in this paper are Ti(C,N)-based nanocomposite cermet mold materials, TiC and TiN are matrix, and ZrO_2, WC, Mo, Ni, C and VC are added phase [6, 7]. The mechanical properties of the ceramic mold material are determined by its microstructure, which is determined by the composition of the material and the sintering process. In the case of the same sintering process, the mechanical properties of the ceramic material can be regarded as it is determined by the content of each component. The experimental data of the mass percentage and mechanical properties of Ti(C,N)-based nanocomposite cermet materials are shown in Table 1. A total of 12 sets of data were obtained under the same hot pressing sintering conditions. The molar ratio of the matrix TiC and TiN in the mass percentage ratio is fixed at 7:3, and the mass percentages of the added phases Mo, Ni, C and VC are fixed [8], and only the phase ZrO_2 and WC are added. The percentage of mass is variable, that is, the change of the two components causes the mechanical properties of the Ti(C,N)-based nanocomposite cermet material.

Mathematical model of stepwise regression analysis method:

Set the x_n dependent variable, x_1, x_2, ..., x_{n-1} to be $n-1$ independent variables (factors). Then the regression equation can be expressed as:

$$x_n = \beta_0 + \beta_1 x_1 + \ldots + \beta_{n-1} x_{n-1}. \qquad (1)$$

The regression coefficient (β_0, β_1, ..., β_{n-1}) is determined by known experimental data, and the F test is performed on each factor, and the factors that do not meet the condition are eliminated, thereby finally determining the functional relationship between the independent variable and the dependent variable, and the features to implement stepwise regression analysis.

Table 1. Percent content and mechanical properties of Ti(C,N)-based nanocomposite cermets

Group	WtTiC, %	WtTiN, %	WtZrO2, %	WtWC, %	WtMo, %	WtNi, %	WtC, %	WtVC, %	σ, %	H, %	KIC
1	54.4	24.0	0	0	7	13	0.8	0.8	980	15.57	6.14
2	51.0	22.6	0	4.8	7	13	0.8	0.8	1001	14.84	5.11
3	47.7	21.1	0	9.6	7	13	0.8	0.8	917	14.92	5.3
4	50.9	22.5	5	0	7	13	0.8	0.8	707	14.71	5.47
5	47.6	21.0	5	4.8	7	13	0.8	0.8	857	15.02	5.60
6	44.2	19.6	5	9.6	7	13	0.8	0.8	1014	15.57	7.25
7	47.4	21.0	10	0	7	13	0.8	0.8	904	14.89	6.44
8	44.1	19.5	10	4.8	7	13	0.8	0.8	706	14.62	6.48
9	40.8	18.0	10	9.6	7	13	0.8	0.8	778	15.30	6.00
10	44.0	19.4	15	0	7	13	0.8	0.8	728	13.57	7.05
11	40.6	18.0	15	4.8	7	13	0.8	0.8	779	14.30	7.01
12	37.3	16.5	15	9.6	7	13	0.8	0.8	748	13.99	5.85

Table 2. Selection of independent variables

No.	I.V.	No.	I.V.	No.	I.V.	No.	I.V.
1	M1	4	M22	7	(M1M2)2	10	e M1
2	M2	5	M1M2	8	Ln(1+M1)	11	e M2
3	M12	6	M1M2 (M1-M2)	9	Ln(1+M2)		

Determination of the objective function of immune algorithm

Since the molar ratio of the matrix TiC and TiN in the Ti(C,N)-based nanocomposite cermet material composition is fixed at 7:3, only the mass percentage of ZrO_2 and WC in the additive phase is changed, and other added phases are added. The mass percentage remained unchanged, so the mass percentages of ZrO_2 and WC were selected as independent variables and set to M1 and M2, respectively. In order to make the selection range larger, the function fitting accuracy is higher, and the two sets of independent variables are expanded into 11 sets of independent variables [9], as shown in Table 2.

The fitting process first linearizes the 11 sets of nonlinear conditions as follows:

$$x_1 = M_1, \ldots, x_1 = M_2^2, \ldots, x_{11} = e^{M^2}. \quad (2)$$

According to the conversion relationship in the above formula, the mass percentages of ZrO_2 and WC, that is, M1 and M2, are transformed into 11 groups of variables. The relationship between fracture toughness and 11 groups of variables is as follows:

$$K_{IC} = a_0 + a_1 x_1 + \ldots + a_n x_n. \quad (3)$$

In the formula, x_n corresponds to the previous 11 sets of variables, and a_0 is the regression coefficient, where n = 11. Enter the values of 11 sets of variables and fracture toughness into the workspace and save them in MATLAB software, then run the stepwise function to obtain the regression coefficient, bring in the equation (3) and restore the variables, and obtain the fracture toughness and ZrO_2 and WC. The mathematical function relationship between mass percentages is as follows:

$$K_{IC} = 15.8 - 958.91 M_1 M_2 (M_1 - M_2) + 15.32 \ln(1 + M_1) - 10.39 e^{M^1}, \quad (4)$$

In the process of stepwise regression analysis, the F-test coefficient of the above formula is $F = 3.71$, and the corresponding significance level is $p = 0.0612$. Therefore, the mathematical model of this function can reflect the fracture of Ti(C,N)-based nanocomposite cermet mold material. The mapping relationship between toughness and components can be used as the objective function of the immune algorithm.

Selection of parameters related to immune algorithm

In the process of optimizing the fracture toughness of Ti(C,N)-based nanocomposite

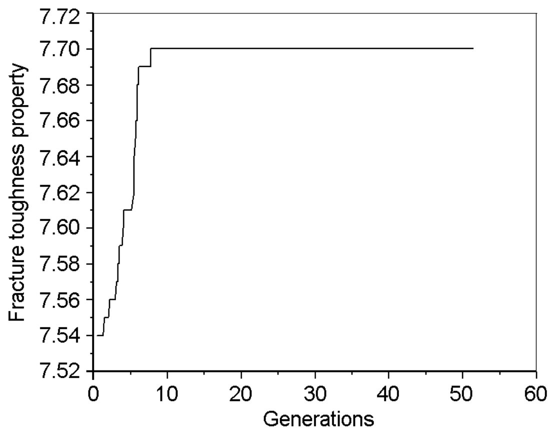

Fig. 1. Immune algorithm optimization fracture toughness fitness curve.

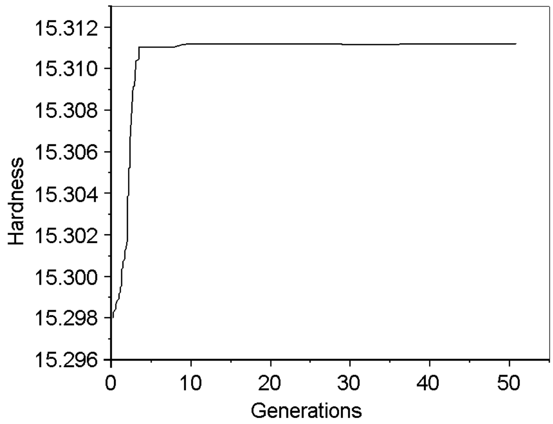

Fig. 2. The fitness curve of the optimized hardness of the immune algorithm.

cermet materials by using immune algorithm, the coding methods of antigens and antibodies are binary coded [10], it is convenient to calculate the affinity between the antibody and the antigen as well as the diversity of the antibody. The parameters of the immune algorithm are set as follows:

Gen = 50, the maximum number of iterations is 50; $P = 100$, the maximum population is 100; $p_m = 0.05$, and the mutation probability is set to 0.05.

The M file is built in the MATLAB software, and the program of each part of the immune algorithm is compiled according to the algorithm flow chart in Fig. 1, then the formula (4) is used as the objective function of the immune algorithm, and the related parameters such as the mutation probability and the maximum number of iterations are set. After the debugging procedure is correct, the running program obtains the optimum value of the fracture toughness and obtains the corresponding mass percentage of ZrO_2 and WC.

2.2 Mathematical model between hardness and flexural strength and composition of nano-composite cermet mold materials

The mathematical relationship between hardness and flexural strength and composition of Ti(C,N)-based nanocomposite cermets is also based on stepwise regression analysis [11], which is the same as the process of establishing the relationship between fracture toughness and the obtained function. The relationship is as follows:

$$H = 15.31 - 66.86M_1^2 + 1067.93M_1M_2(M_1 - M_2), \quad (5)$$

$$\sigma = 1157.39 - 18408.5M_1^2 + 18243.6M_1M_2 - 3124.31\ln(1 + M_2). \quad (6)$$

While using stepwise regression analysis to establish a functional relationship between hardness and flexural strength and composition, F test is also performed on equations (5) and (6), respectively, and the F-test quantities are $F = 6.63$ and F=12.26, respectively, the corresponding significance levels are $p = 0.017$ and $p = 0.0023$, respectively, so the functional relations of equations (5) and (6) can reflect the hardness and resistance of Ti(C,N)-based nanocomposite cermet materials. The mapping relationship between bending strength and components can be used as an objective function of the immune algorithm. The main program of the immune algorithm is the same as the optimized fracture toughness. The same parameters are also used for each parameter. Equations (5) and (6) are used as the objective functions of the immune algorithm, and the Ti(C,N)-based nanocomposite cermet mold is applied. The hardness and flexural strength of the material were optimized by an immune algorithm to obtain the optimum values of hardness and flexural strength, and the corresponding mass percentages of ZrO_2 and WC.

The immune genetic algorithm was applied to the optimization design of Ti(C,N)-based nanocomposite cermet mold components. Since the composition of the materials is the same, the mechanical properties (fracture toughness, flexural strength and hardness) and the mathematical model between the components are the same in the algorithm optimization process. The objective function of the algorithm is also stepwisely regressed in Chapter 2. The analytical method is the same.

Create M files in MATLAB software and program the sub-functions of the immune genetic algorithm. The antigen and antibody

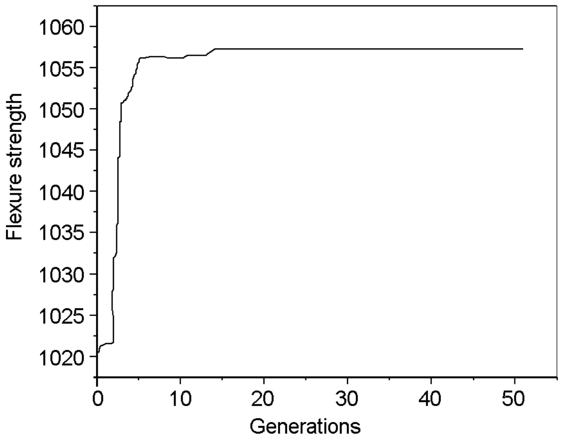

Fig. 3. The fitness curve of the immune algorithm to optimize the flexural strength.

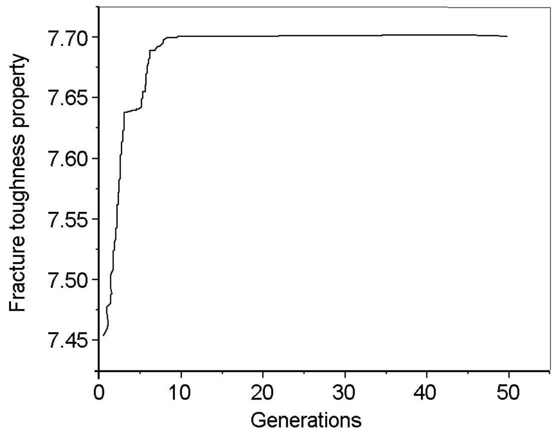

Fig. 4. Immune genetic algorithm to optimize fracture toughness fitness curve.

in the algorithm are also binary coded [12], and the parameters are set as follows:

$P = 100$, the maximum population is 100;

$Gen = 50$, the maximum number of iterations is 50;

$P_c = 0.5$, the crossover probability is set to 0.5;

$P_m = 0.01$, the mutation probability is set to 0.01.

The functional relationship between fracture toughness, flexural strength and hardness in formula (4), formula (5) and formula (6) and Ti(C,N)-based nanocomposite metal nanomaterials is used as immune genetic algorithm. The objective function, after running the program respectively, obtains the optimal values of fracture toughness, flexural strength and hardness, and at the same time obtains the group distribution ratio corresponding to each optimal value.

3. Result analysis

3.1 Immunization optimization results

The optimization results of the immune algorithm are shown in Fig. 3 to Fig. 5. The optimum value of fracture toughness is 7.7 MPa·m$^{1/2}$, and the corresponding mass percentages of ZrO_2 and WC are 10.67 % and 20 %. The optimum hardness value is 15.31 GPa, and the corresponding mass percentages of ZrO_2 and WC are 0 and 15.10 %. The optimum value of the flexural strength is 1057.39 MPa, and the corresponding mass percentages of ZrO_2 and WC are 6.75 % and 11.38 %.

It can be seen from the variation curve of the fitness value in the optimization process of the immune algorithm in Fig. 3, Fig. 4 and Fig. 5 that the immune algorithm is running in the optimization process of the mechanical properties of the Ti(C,N) based nanocomposite cermet material. It converges around 20 generations and gets the global optimal value. Although the algorithm will have an inflection point during the convergence process, as shown in Fig. 3, running to the 8th generation, Fi. 4 running to the 5th generation, and Fig. 5 running to the 6th generation, these inflection points are local minimum points, but the algorithm is not in these The inflection point converges, but skips these local best points, converges to a larger global best, without premature convergence. It is indicated that the immune algorithm is feasible for the optimization design of Ti(C,N)-based nanocomposite cermet material components.

3.2 Results of immune genetic algorithm optimization

Figures 4, 5 and 6 correspond to the change trend of the fitness curve in the process of optimizing the fracture toughness, hardness and flexural strength of the immune genetic algorithm. When the fitness is not changing, the algorithm converges to the global optimum. It can be seen from the fitness change graph that the algorithm has a partial inflection point in the convergence process, but the algorithm does not converge to these local optimal values, but converges to the global optimal value. According to the optimization results of immune genetic algorithm, the optimal value of fracture toughness is 7.7 MPa·m$^{1/2}$, and the corresponding mass percentages of ZrO_2 and WC are 10.63 % and 20 %; the optimum hardness is 15.31 GPa. The corresponding mass percentages of ZrO_2 and WC are 0 and 14.86 %; the optimum value of flexural strength is 1057.39 MPa, and the

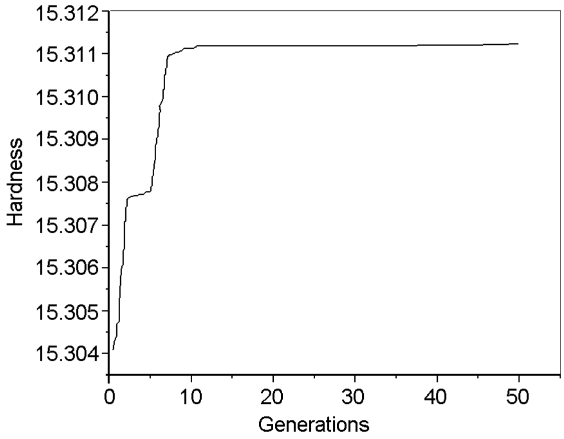

Fig. 5. Fitness curve of immune genetic algorithm to optimize hardness.

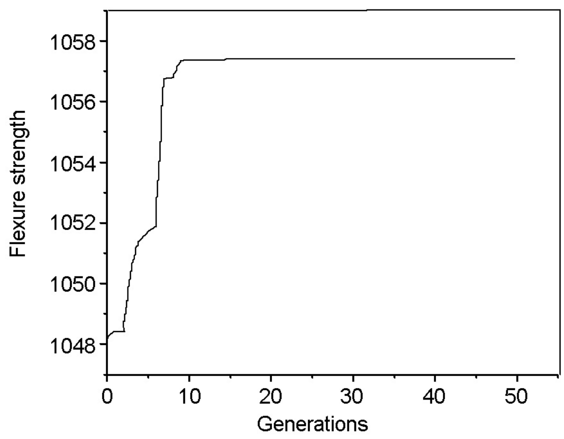

Fig. 6. Fitness curve of immune genetic algorithm optimizes bending strength.

corresponding mass percentages of ZrO_2 and WC are 5.86 % and 10.59 %.

Immune genetic algorithm and immune algorithm converge to the same global optimal value in the optimization process, and neither of the two methods have local convergence and premature convergence, but in the optimization process of fracture toughness, hardness and flexural strength, immunity The number of iterations of the genetic algorithm is significantly reduced compared to the single immune algorithm. In Fig. 4, the immune algorithm converges in the 12th generation, and the immune genetic algorithm converges in the 8th generation. In Fig. 5, the immune algorithm converges in the 10th generation, and the immune genetic algorithm In the sixth generation convergence; in Fig. 6, the immune algorithm converges in the 16th generation, the immune genetic algorithm converges in the 10th generation, and the convergence speed of the immune genetic algorithm increases by 50 %, 40 %, and 37.5 %, thereby further improving Ti(C,N) based nanocomposite metal nano-mold material composition optimization design efficiency.

3. Conclusions

The mechanical properties of Ti(C,N)-based nanocomposite cermets were optimized by immunogenetic algorithm, and the corresponding material components were obtained. The optimization results are: the optimal value of fracture toughness is 7.7 MPa·m$^{1/2}$, the corresponding mass percentages of ZrO_2 and WC are 10.67 % and 20 %; the optimum hardness is 15.31 GPa, corresponding to ZrO_2 The mass percentages of WC and WC are 0 and 14.86 %; the optimum value of flexural strength is 1057.39 MPa, and the corresponding mass percentages of ZrO_2 and WC are 5.86 % and 10.59 %. The algorithm converges to the same global optimal value in the optimization process, and there is no problem of premature convergence and local convergence. However, in the optimization process of fracture toughness, hardness and flexural strength, the number of iterations of immune genetic algorithm is significantly reduced. Comparing the optimization results of immune algorithm and immune genetic algorithm, The convergence rate of immune genetic algorithm is faster than immune algorithm, and the optimal composition is obtained, which improves the efficiency of ceramic mold material design.

References

1. Z.Jie, T.Min, in: Proc. of Intern. Conf. on Image (2017).
2. L.Zhu, X.Guo, H.Ruan, *Compos. Sci. Techn.*, **123**, 222 (2016).
3. L.H.Ma, H.B.Wang, B.Y.Fang, *Colloids Surf. B Biointerfaces*, **162**, S0927776517308512 (2017).
4. Q.Wang, *Functional Materials*, **26**, 615 (2019).
5. M.Arshadi, F.Mousavinia, M.J.Amiri, *J. Colloid Interf. Sci.*, **483**, 118 (2016).
6. N.N.M.Zawawi, W.H.Azmi, A.A.M.Redhwan, *Intern. J. Refrigeration*, **89**, S0140700718300483 (2018).
7. B.R.Vishnu, S.K.Kanta, S.K.Albert, *Process Safety & Environmental Protection*, 114 (2018).
8. M.Zhang, S.Zhan, Z.He, *Mater. Design*, (2017).
9. M.Khan, S.K.Misra, Z.Wang, *Analyt. Chem.*, **89**, 2107 (2017).
10. C.Meng, X.Zhi, C.Li. *Acs Nano*, **10**, 2203 (2016).
11. E.A.Scott, N.B.Karabin, P.Augsornworawat, *Ann. Rev. Biomed. Engin.*, **19**, (2017).
12. S.Manzo, S.Schiavo, M.Oliviero, *Sci. Total Environ.*, **599**, 9 (2017).