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An artificial neural network model of the chemical vapor deposition processes for carbon – carbon composites

Jianguo Zhao*, Yong Guo, Feng Feng, Jinsheng Jia, Xiaojun Yuan, Wanhua Xue, Haiqing Wang

Institute of Carbon Materials Science, Shanxi Datong University, Datong, 037009, P. R. China.

A model of artificial neural network (ANN) is developed for the analysis of the correlation between the chemical vapor deposition (CVD) processing parameters and the densification of carbon - carbon (C/C) composites. The input parameters of the ANN model are the manipulative temperature, the density of carbon fiber preforms and the flow rate of acetylene. The output of the ANN model is the density of C/C composites. With the aid of the ANN model, the effects of the CVD processing parameters on the densification of C/C composites are discussed and the relationship between the process conditions and the microstructure of pyrocarbon is discussed as well.

Keywords : Carbon - carbon composites, Chemical vapor deposition; Microstructures; Artificial neural network.

1. Introduction :

C/C composites are not only of outstanding high temperature performance carbon materials, but also retain excellent mechanical performance of composites. Their advantages include low densities, chemical resistance, high thermal conductivity, high heat capacities, good resistance to thermal shock, excellent high-temperature friction and wear characteristics and biocompatibility. They have been used successfully in the field of aerospace for the last three decades. Despite of their attractive properties, the development of C/C composites is severely limited because the materials are extremely expensive due to the inefficient fabrication processes being used currently. Due to expensive and time consuming fabrication process of C/C composites, optimized parameters are difficult to obtain. The nonlinear correlation between these parameters and physical properties is too complex to be described by the physical models. In fact, the process parameters are empirical in nature and still the method of trial and error is common and considered best suited [1, 2]. ANN with artificial intelligence is a kind of computer emulational system. ANN caters for dealing with sophisticated multidimensional nonlinear problems. ANN does not need any physical models. According to assured computational rule after many iterative trains, the ANN model can be established, which can reflect the intrinsic law among sample data. This successfully trained ANN model can quickly forecast the accurate result for the unknown sample data. Therefore, ANN is used widely in the fields of material processing and design [3]. In this paper, a model of ANN is developed for the analysis and prediction of the correlation between the chemical vapor deposition (CVD) processing parameters and the densification of C/C composites. Moreover, the effects of the CVD processing parameters on the densification of C/C composites and the microstructure of pyrocarbon are studied.

2. Experimental :

Preforms used in this study are carbon fiber felts. The apparent density of preforms is between 0.2 - 0.85 g/cm^3. The densification of porous carbon fiber felt is performed in a CVD furnace, which is an electrical furnace equipped with a horizontal quartz tube 50 mm in diameter, 1000 mm in length and a 150 mm long reaction zone in the middle. The preforms was put on the porcelain boat, which was moved into the middle part of the CVD furnace, and heated up to 1000 C within 5 h under the protection of argon gas. Then acetylene was introduced into the furnace as carbon source, nitrogen as dilute and carrier gas. The temperature in the deposition region is manipulated between 900 C – 1200 C and monitored by a Pt-Rh type thermocouple. The entire CVD process runs at ambient pressure. The flow rate of acetylene is controlled between 1.6 - 3.5 ml/sec. The texture of the infiltrated pyrocarbon is characterized with polarized-light microscopy.

3. Establishment of ANN model :

3.1 Back Propagation Neural Network :

The back propagation (BP) neural network is well known in the world. ANN consists of parallel working neurons, and the information of sample data is deposited in the connection joints. An example of a neuron with a sigmoidal transfer function is shown in Figure (1).

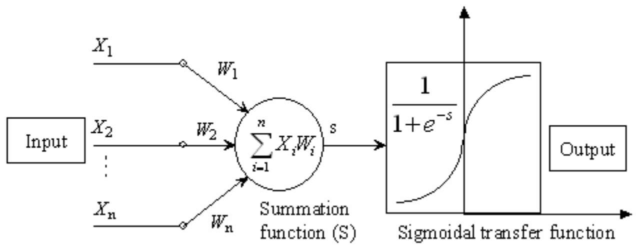


Figure (1) : A neuron with a sigmoidal transfer function

The classical training algorithm of ANN is the steepest descent one, which often converges too slow near the extremum point of the objective function and is easy to relapse into local minimum for practical problems. Therefore, a lot of improved methods are suggested. Gauss-Newton methods are less complicated because only one step differential coefficient is employed. However, in practice the Gauss-Newton formula is not always stable, which is improved by Levenberg-Marquardt methods through adding a modifying value. Morbid matrix is well disposed in the modified Gauss-Newton formula. The later methods are of good stabilization and become the standard method of numerical optimization techniques. In this paper, Levenberg–Marquardt algorithm is adopted in ANN of the CVD for C/C composites [4].

3.2 Collecting sample data :

In the ANN of the CVD for C/C composites, teaching samples are the impersonal carrier of the intrinsic law which is contained among processing parameters. Its magnitude and distribution severely affect the precision and the generalization. In nature, ANN is suitable for the insert operation, but not for extrapolating operation. Therefore, in this paper the sample data cover the whole experimental range. The temperature is the main factor which affects the pyrolysis reactions of acetylene. According to the Arrhenius equation, the rate constant of chemical reaction increases exponentially with the increasing of temperature [1]. In this ANN, the processing parameter of manipulative temperature is designed with four levels, 900 C, 1000 C, 1100 C, and 1200 C. Carbon fiber preforms are the physical base of the microcosmic environment of pyrocarbon deposition. Preforms manipulate the active surface area and channels for the precursor to pass and diffuse in the processing of chemical vapor deposition. So the preforms density is designed with eight levels, 0.2 g/cm^3, 0.4 g/cm^3, 0.45 g/cm^3, 0.50 g/cm^3, 0.55 g/cm^3, 0.60 g/cm^3, 0.65 g/cm^3, and 0.85 g/cm^3. The flow rate of acetylene is another important parameter for CVD process. Acetylene is introduced into the preforms by diffusion in the CVD process. The optimal flow rate can ensure the steady concentration and eliminate the influence of precursor on the pyrocarbon deposition. Thus seven levels, 1.6 ml/sec, 2.0 ml/sec, 2.4 ml/sec, 2.7 ml/sec, 3.0 ml/sec, 3.3 ml/sec, and 3.6 ml/sec are selected in this paper. The entire CVD process runs at ambient pressure. In this study, only the manipulative temperature, the density of carbon fiber felt, and the flow rate of acetylene are chosen as the input parameters to simplify the complicated processes. The density of C/C composites is the main quality index and it is picked as the output parameter.

3.3 The framework of ANN :

The hidden layers of the ANN work as a 'Black Box'. They can mine the impersonal law of the sample data and deposit this law in the ANN framework. They influence the generalization capability and reliability of the ANN. The hidden layers consist of one or more layers. The more layers the ANNs possess, the more precise the ANNs are. However, the operation calculation rate of the ANNs is slower. Therefore, the number of the hidden layers is reasonably designed in accordance with the computation velocity and the precision. The number of neurons of the hidden layers is related to the precision. Theoretically, the more number of neurons the hidden layers possess, the less errors the system have, which will result in an interminable computation.

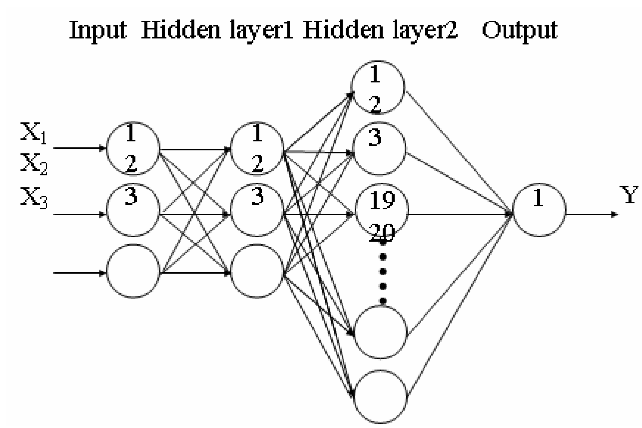


Figure (2) : The four-layered feed-forward neural network

The number of neuron of hidden layers has great effects on the structure and the performance of ANNs. So far, there has not been any theory for the establishment of the number of neuron of the hidden layers except depending on the work experience and trials. In this model, two hidden layers are selected, three neurons in the first hidden layer, and twenty neurons in the second hidden layer. In other words, there are three neurons in the input layer and one neuron in the output layer. The procedure is shown schematically in Figure (2).

3.4 Training the ANN model and testing generalization

This ANN model is trained in the computer with Intel Pentium IV 2.4G CPU. The sum of squared errors (SEE) criterion of the system is set at 0.01. After 200 iterations of 90 teaching samples the SSE of the system is less than 0.01. Figure (3) shows that the predicted outputs of 12 testing samples conform favorably to the desired output values, indicating that the ANN model is accurate enough to produce good generalization. This model can be used for mining the impersonal information in data. It can obtain the desired values for the unknown samples data and is suitable for analysis and study of the CVD for C/C composites.

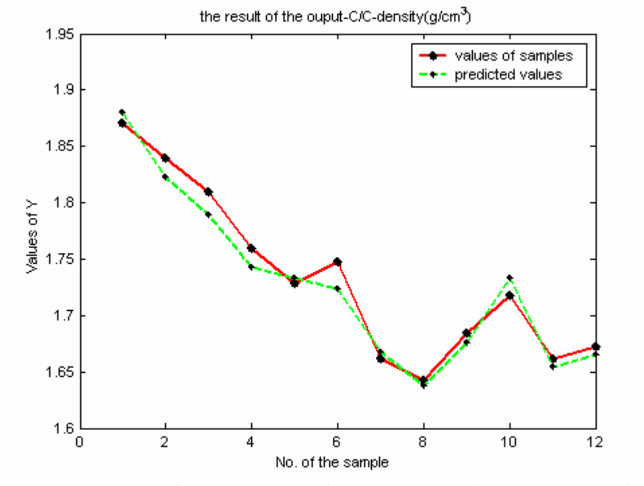


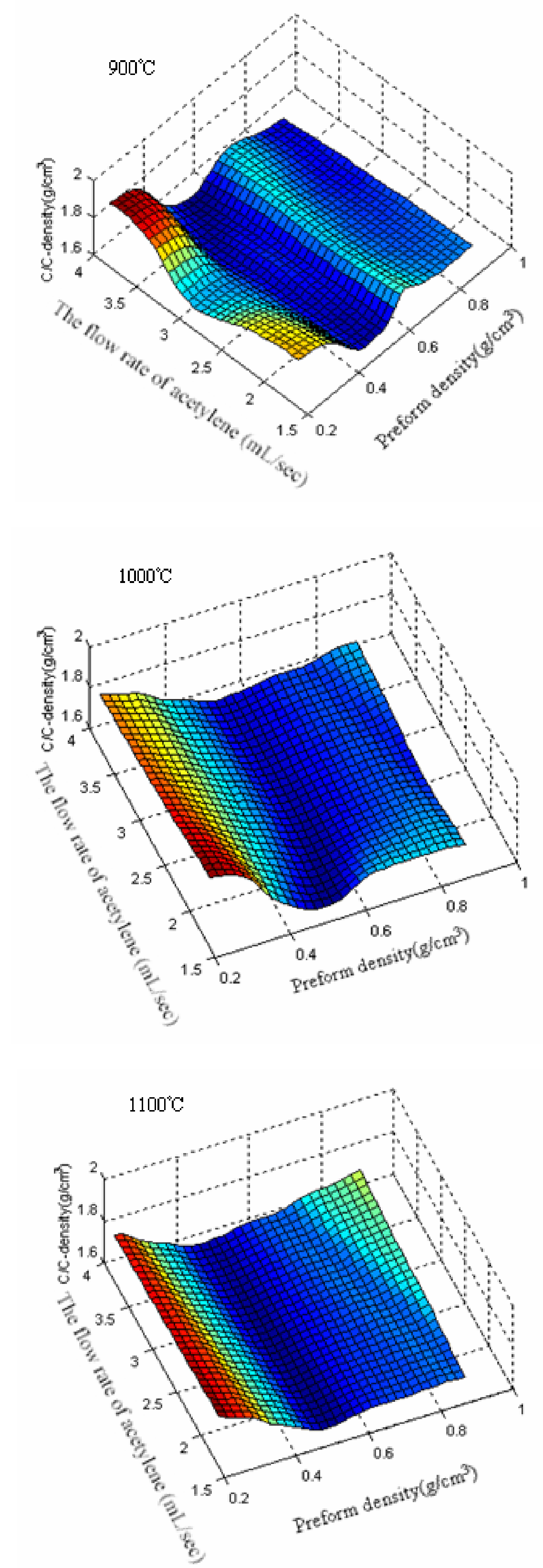
Figure (3) : Testing results of the generalization of the neural network

4. Results and Discussion :

This well-trained ANN model can not only present the forecast values for the unknown sample data and realize the aim of doing experiments with computer, but also analyze the relationship among processing parameters and show the internal law in the sample data. With the help of this model, the principle of the CVD process of C/C composites is easily accepted and the processing parameters may be optimized. Three-dimensional graphs are used to explain the effects of the CVD processing parameters on the densification of C/C composites.

4.1 Effect of manipulative temperature on densification

When the manipulative temperatures are 900 C, 1000 C, 1100 C, and 1200 C respectively, Figure (4) indicates the influence of the density of the preforms and the flow rate of acetylene on densification of C/C composites. With preform density of 0.2 g/cm^3, the C/C composites have the highest density at all manipulative temperatures. The partial reason is that C/C composites consist of carbon fiber and pyrocarbon, and carbon fiber density is about 1.75 g/cm^3, and the density of pyrocarbon is nearly 2.2 g/cm^3. So, the fewer carbon fiber fraction is, the higher density C/C composites possess. Figure (4) shows the flow rate of acetylene has little effect on the densification of C/C composites. The density of the preforms has significant effects on the densification of C/C composites at manipulative temperatures of 1000 C, 1100 C, and 1200 C. When the manipulative temperature is 900 C, the high density C/C composites can be achieved under the high flow rate of acetylene. When the manipulative temperature is 1200 C, the high density C/C composites can be fabricated under the high flow rate of acetylene and the high density preforms. When the manipulative temperature is 1000 C, 1100 C, and 1200 C respectively, three-dimensional graphs are similar. The reason is that the rate of chemical vapor deposition reaction increases exponentially with the increasing of temperatures **[1, 5]**. After the temperature is over 900 C, the influence of chemical kinetics on chemical vapor deposition reaction is minimized while the influence of acetylene concentration inside the hot deposition zone on that is maximized.



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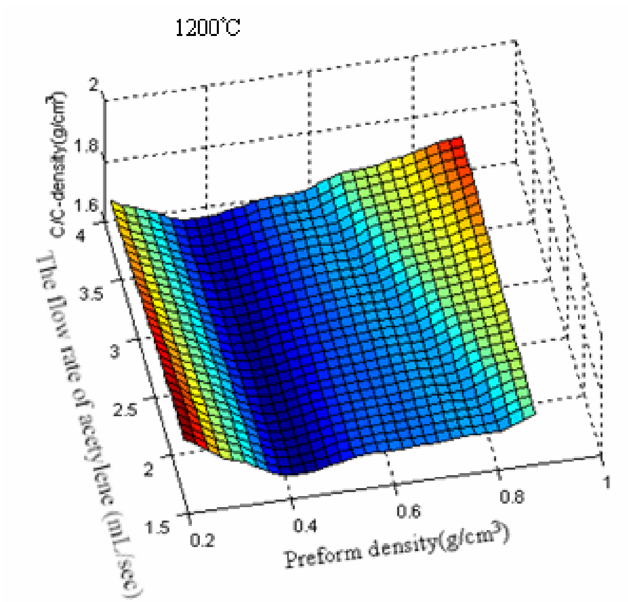
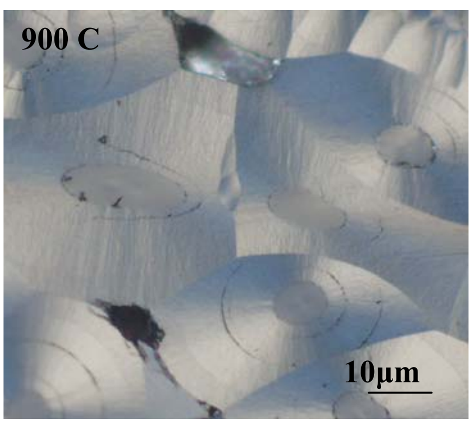
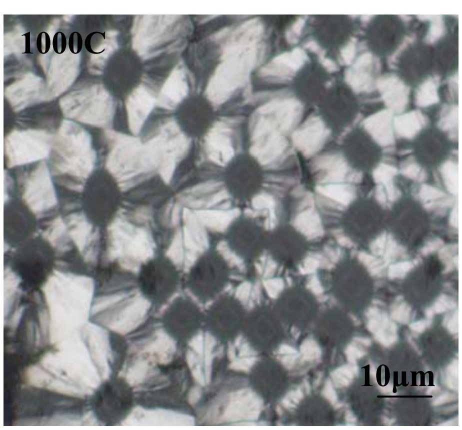


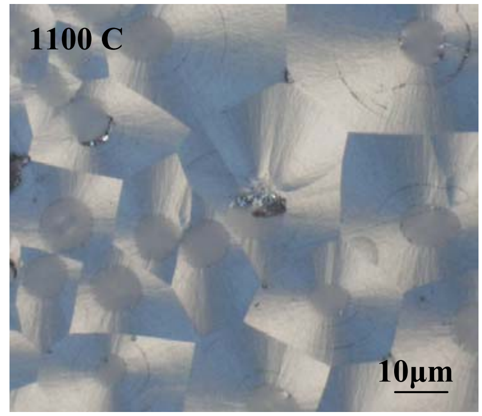
Figure (4) : The three-dimensional map of the flow rate of acetylene, the density of preforms and the density of C/C composites when the manipulated temperature is 900 C, 1000 C, 1100 C, and 1200 C.

4.2 Influence of manipulative temperature on microstructure of pyrocarbon :

When the preform density is 0.2 g/cm^3 and the flow rate of acetylene is 1.6 ml/sec, the influence of the manipulative temperature on the micro-structure of C/C composites is shown in Figure (5).







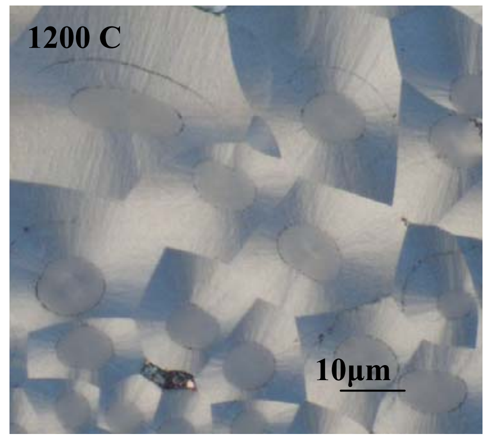
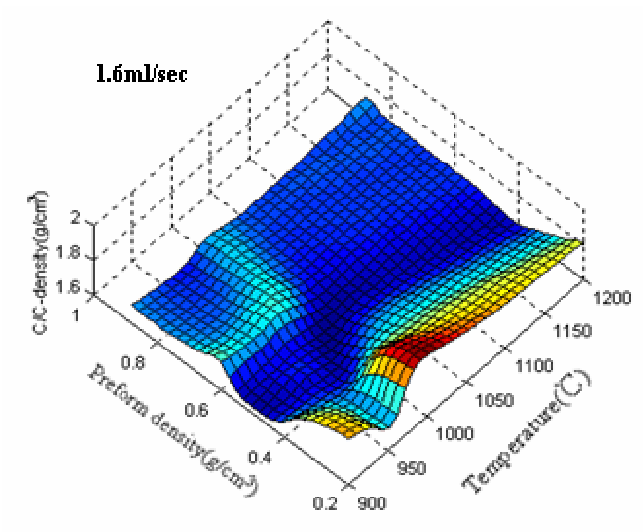


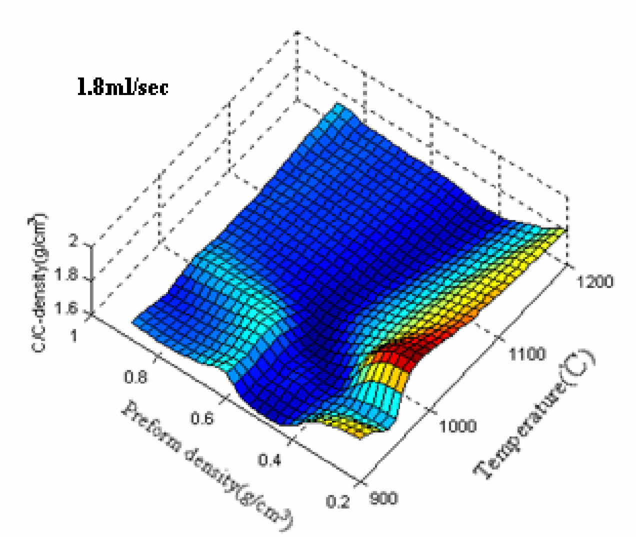
Figure (5) : The effect of manipulative temperature on microstructure of pyrocarbon when preform density is 0.2 g/cm^3 and acetylene flow rate is 1.6 ml/sec.

It is obvious that the rough laminar pyrocarbon can be seen at 1000 C, and the smooth laminar pyrocarbon at 900 C, 1100 C, and 1200 C. At a given value of the preforms density and the flow rate of acetylene, acetylene concentration at the deposition region will be stable. Therefore, the temperature becomes the main factor. Research on chemical dynamics of chemical vapor deposition demonstrates that the deposition reaction is extremely complex and composed of several consecutive and parallel reactions. Dominating growth species of pyrocarbon include small linear hydrocarbons and larger polycyclic aromatic hydrocarbons (PAHs). The high–textured pyrocarbon is formed from a gas phase with an optimum ratio of aromatic to small linear hydrocarbons. The low – textured pyrocarbon such as smooth laminar pyrocarbon and isotropic pyrocarbon is produced from a gas phase with an excess of aromatic or small linear hydrocarbons [1, 5]. When the pyrolysis temperature increases, the gas phase reactions are progressively favored, leading to an excess of small linear hydrocarbons species. These small species partially combine into larger species polycyclic aromatic hydrocarbons from undergoing aryl-aryl combination and intramolecular dehydrocylization reactions, and partially form pyrocarbon. With the increasing of temperature, the ratio of aromatic to small linear hydrocarbons increases. At 1000 C, the optimum ratio can be gained with the high-textured rough laminar pyrocarbon being formed.

4.3 Influence of acetylene flow rate on densification :

Figure (6) shows the effect of the manipulative temperature and the density of preforms on densification of C/C composites when the flow rates of acetylene are 1.6 ml/sec, 1.8 ml/sec, 2.5 ml/sec, and 3.0 ml/sec respectively. It can be seen that the flow rate of acetylene has less influence on densification than manipulative temperature and preform density. The entire CVD process runs at ambient pressure during the course of experiments. The efficient utilized ratio of acetylene is about 25 %. So the concentration of acetylene in the reaction furnace keeps steady and the change of acetylene flow rate has little effect on densification. In addition, the density of C/C composites is the highest under different flow rates of acetylene when the manipulative temperature is 1000 C and the density of the preform is 0.2 g/cm^3. This result agrees well with the rough laminar carbon in Figure (5) obtained under the same condition.





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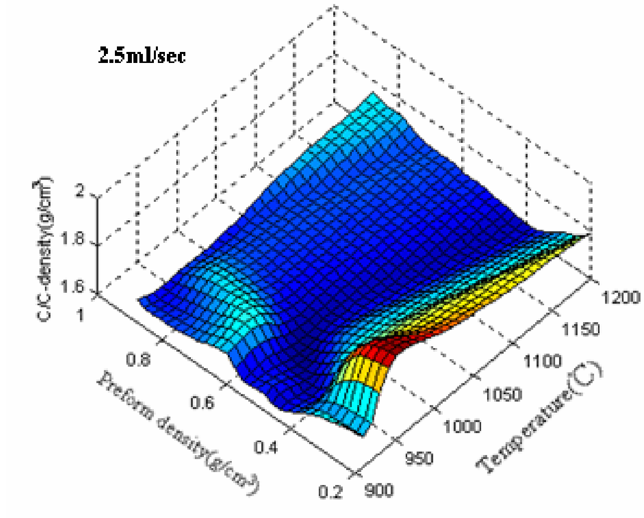

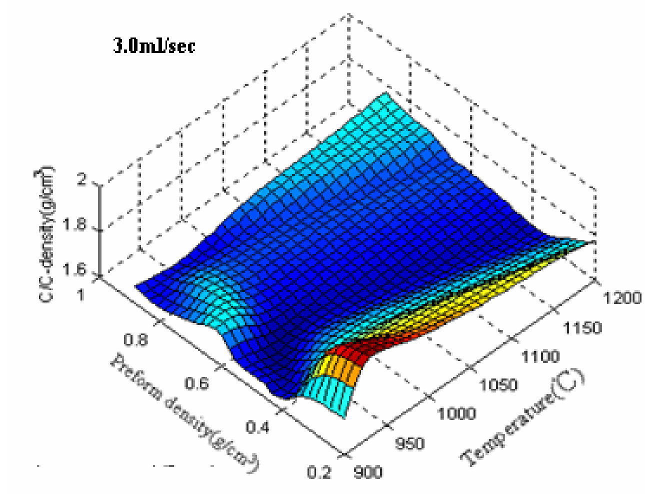

Figure (6) : The three-dimensional map of the manipulated temperature, the density of preforms and the density of C/C composites when acetylene flow rate is 1.6 ml/sec, 1.8 ml/sec, 2.5 ml/sec, 3.0 ml/sec

5. Conclusions :

（1） The model of ANN of the CVD for C/C composites can reflect the relationship between the processing parameters and densification of C/C composites. It can be a useful guidance towards the process optimization.

（2） The manipulative temperature and the density of preform exert more significant impact on densification of C/C composites than the flow rate of acetylene.

（3） The high-textured rough laminar pyrocarbon can be obtained at the temperature of 1000 C and the preform density of 0.2 g/cm^3.

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