

THE NEURAL NETWORK MODEL FOR CVD PROCESS OF ANTI-OXIDATION COATING ON C/C COMPOSITES

He-Jun Li, Zhi-Huai Xu, Hong-Mei Han, Li-Bao Yang

*Department of Material Science and Engineering, Northwestern Polytechnical University,
Xi'an, 710072, P.R.China*

Introduction

The good mechanical properties and erosion resistance of silicon carbide (SiC) play an important role in enhancing the oxidation resistant ability of carbon/carbon (C/C) composites^[1]. The quality of SiC-coating on the C/C surfaces determines the service life and behavior of C/C high temperature structural parts. Therefore, it is necessary to understand the SiC-CVD process thoroughly. Modeling the SiC-CVD process becomes the key to optimization and intelligent control of oxidation prevent coating fabrication.

At present, the SiC-CVD process model is mainly classified into two kinds^[2]. One is the unstructural model, and the other is the structural model. Basing on the engineering application level, the former model mainly relies on practical operating experience, integrating the presentational description derived from practical process and neglecting the variation of internal structure and composition. While, founded on the understanding of the procedure at molecular level and thorough investigation of internal change in structure and composition, the structural model expresses the deposition process by a series of symbolic equations and finds its way in many laboratory researches. Briefly, establishing the correct structural model needs the deep understanding of practical procedure mechanism, intermediate reactions and their interaction.

Taking no consideration of the internal changes, the unstructural model approximately describes the law of SiC-CVD process. At the time the multi-factors alter, it is incapable to draw correct conclusion of the deposition condition. Meanwhile, the unstructural model has difficulty in attaining the deposition result under certain circumstance, limiting its application in automatic control of fabrication. In contrast, the structural model has an advantage in

reflecting the intrinsic characteristic of the simple procedure. However, as to the complicated practical process with numerous influencing factors and unclear mechanisms, due to the lack of prior knowledge, the model is inevitable to grounded on a considerable simplification, abstraction and hypotheses, leading to the reduced reliability. Making up for these deficiencies, in this paper, the neural network identification theory is adopted in SiC-CVD process modeling.

Procedure Model

On the basis of experimental observation, the complicated SiC-CVD process is thought to comprises such stages as mass transfer, preheating and pre-decomposition, gas decomposition reaction, absorption and de-absorption, agglomeration and growth (shown in Fig.1). In the low air current environment where laminar flow predominates, the mixture and mass transfer of the reactants before the reactions determine the sequent chemistry distribution and growth rate. Preheating and pre-decomposition, influenced greatly by heating patterns, the shape and size of the reactive room and the features of the airflow, refer to heating up and pyrolysing the reactants before their arrival to the deposition surfaces. Considering the sequent reactive directions and practical mechanisms are decided on the pyrolytic resultants, i.e. CHSiCl or $\text{CH}_4+\text{SiCl}_2$, the thorough investigation of this stage is crucial for the reactive room design and the reactive direction control. The reactive processes nearby the depositing surfaces consist of hundreds of chemical reactions taking place among tens of middle products, and only the system $\text{SiCl}_4+\text{CH}_4+\text{H}_2$ gets the fairly clear understanding^[2]. As for other depositing systems, the process investigation is just touched.

Furthermore, the varied component shapes and deposition requirements lead to different surface air current conditions and specific fabrications, which adds difficulty to understand the certain deposition process. Hence, the absorption and desorption in the deposition process are usually neglected. For the growth on SiC surfaces, the mechanisms put forward by the different researchers are not same [3-4].

In view of numerous indefinite factors in CVD process, it still has much room for the improvement on experiments and testing analysis to set up the sound mathematical model. In this paper, adopting the neural network identification technology, basing on a large quantity of process experiments, using neurons of different constructions to describe the primary influencing factors in each deposition phase, and integrating the deposition behaviors, the

appropriate network topologic structure model is developed and reflects the nonlinear relationship between the deposition environment and the deposition result preferably (seeing formula 1).

$$Z = f(g_1(X_1), g_2(X_2), g_3(X_3) \dots) \quad (1)$$

Where Z represents the deposition result, X_1, X_2, X_3 the deposition influencing factors, g_1, g_2, g_3 the nonlinear change of each factor, and f the nonlinear relationship between the deposition environment and the deposition result. Compared with other SiC-CVD procedure models, our model gives prominence to the influences, exerted by mass transfer and pre-decomposition of the reactive gases before their arrival to deposition surfaces, on the deposition process. At the same time, the model emphasizes the decisive effects of certain chemical reactions on the deposition conditions.

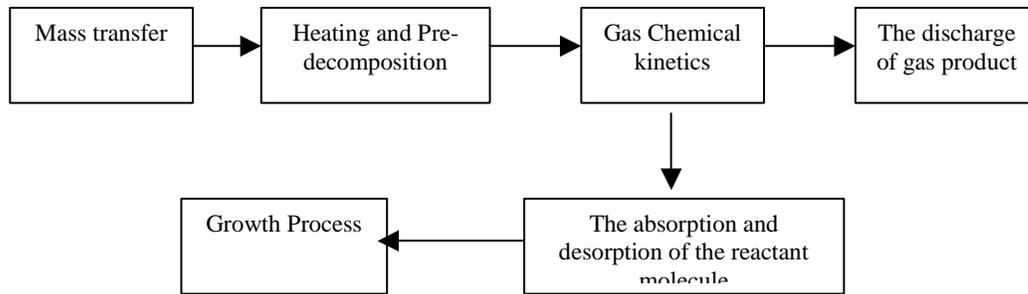


Fig. 1 Schematic of deposition

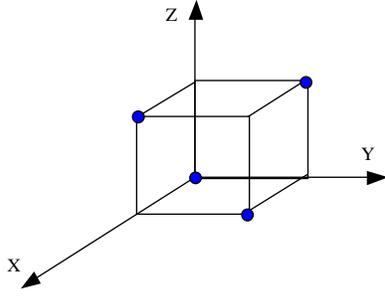
Improvement in Learning Algorithm

In the course of neural network learning, the fastest gradient descent method is adopted and the neuron weight of each layer is adjusted via gaining the least quadratic error gradient of the learning result. In our work, combining the deposition behaviors, improvements have been achieved on the basis of original algorithm.

Design of Orthogonal Learning Sample

The functional capability of the neural network indicates whether the network works reliably. In order to make the trained network quite capable in functionality, that is, the right conclusion can be drawn even for the unknown samples, it is necessary to enlarge the representative learning samples and make them distributed overall. The

orthogonal method, possessing ‘even distribution’ feature in nature [6], provides efficient way to improve the distribution of the learning samples. Because of the orthogonality, it is inevitable for the samples to distribute evenly in the whole sample space. Figure 2 illustrates the locations of $L_4 \times 2^3$ sample nodes in the overall space. Clearly, four sample nodes regularly locate on the six surfaces and twelve edges. Therefore, distribution unevenness of samples is completely got rid of by training the neural network via orthogonal samples. As a result, the network describes the deposition process totally, enhancing the reliability of the model.



Network Structure and Adaptive Regulation of Learning Parameter

According to Kolmogorov law, any successive function can be accomplished via a three-layer forward network. Nevertheless, no feasible method is offered to construct a network. Hence, in practical operation, the trial and error basing on error crossover evaluation is generally applied in selection of network structure and learning parameters. In this paper, a network neuron auto-generation method is put forward to adjust the network structure automatically. During the learning course, the network structure is regulated dynamically by the change of overall error. In the meantime, the parameters, such as learning step and momentum coefficient, must be regulated simultaneously to avoid the unsteady, or even diverge, of the learning process. Thus, some improvements have been made on specific learning procedure resulting in the adaptive regulation of learning parameters. The algorithm can be described as follows:

Imagine each number of n procedures a learning stage, the error of the n -time learning is E_n , the error variable of the first stage is $\square E_1$, and the error variable of the k -time learning procedure is $\square E_k$. Therefore,

When $E_n \leq \epsilon$, if $\square E_k \square \square E_{k-1} \square \square E_k \square \sigma$,

then $I \square I+1 \square$

When $E_n \geq \epsilon$, if $\square E_k \square \square E_{k-1} \square \square E_k \square \sigma$,

then $\alpha \square \eta_1 \alpha$ and $\beta = \eta_2 \beta$.

Where, ϵ , σ , η_1 , η_2 represent the regulation coefficients of network, I the neuron number of the hidden layers, and α ,

β the step and momentum coefficient respectively.

Results and Discussions

The judgement on interaction of process factors

The promotion or counteraction of the testing results, occurring in the experiments when the different factors are arranged in pairs, consists of one of the primary elements that must be taken into account in the experiment planning. Whether the interaction exists among each procedure element depends on the practical experience of the operator in great degree. There, to the complex experiments with multi- influencing factors of varied level, it is extremely difficult to define the interaction.

Fig.3 displays the influence of Ar flow on the SiC-coating thickness under the different pretreatments and H_2 flows. In the case of the H_2 flows change, the relationship between the Ar flow and the coating thickness becomes distinguished (Fig.3-a). When the H_2 flow is less than 300ml/min, the coating thickens firstly followed by thins out as the Ar flow increases. And when the H_2 flow is up to 600ml/min, the coating thickness reduces linearly with the increase of Ar flow. On the other hand, as shown in Fig.3-b, to the varied pretreatments, the coating thins out in similar linear as the Ar flow increases. Despite the coating thickness varies, its relationship to the Ar flow keeps consistent on the whole.

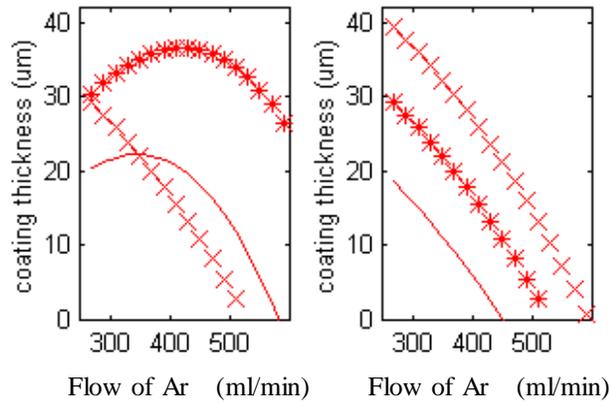
It is inferred from the above consequences that at the time H_2 flow alters, the Ar flow and coating thickness interaction rule turns into inconsistent, as well as the Ar flow influencing extent on the coating thickness. On the other hand, despite the varied pretreatments change the extent of Ar flow effect on coating thickness, the interaction between the coating thickness and Ar flow keeps in the invariable rule. It goes without saying that the Ar carrier gas flow in reactions exhibits no interaction with the pretreatment prior to the deposition, but however shows distinct interaction with the H_2 reductive gas flow.

Due to its native inertness, the argon influences the deposition process by changing the mass transfer and heat conduct in the reactive room, the density of the reactants, the reactant retention time in the furnace, and the thickness

of the boundary. So, it is inferred that the argon certainly exists an interaction with H_2 flow, which behaves similarly but in varying degree. Meanwhile, owing to no surface reactions involved, the argon shows no interaction with the pretreatment, which aims at altering the material surface condition. As to the details of the interaction between Ar

and H_2 , it remains to be investigated further.

In a brief, it is straightforward and physically clear to analyze the interaction among procedure factors by the neural network model, providing a new access to interaction analysis of complicated experiments.



Time Effect

As the deposition process goes on, the density distribution of gaseous phase near the substrate surfaces and the constitution of material itself change continuously. Consequently, the practical procedure and the mechanism of deposition vary with the time. Fig.4 exhibits the time effects on deposition rate under various Ar flows. As can be seen from Fig.4, in the case of other parameters keep constant, the deposition speeds to a peak value before slows down as the deposition time lasting. However, it is noted that curves under different Ar flows exhibit variation. Specifically, the higher deposition rate can be achieved at smaller Ar flow, and the time for deposition rate to attain its peak becomes shorter. The contrary is the case at large Ar flow.

In the course of SiC deposition, the deposition rate is mainly affected in two ways. Firstly, in order to grow, SiC need to eliminate the dissimilarity of lattice constant and physical-chemical behavior with the substrate material. Next, with the deposition time lasting, the density of HCl in

the reactor increases, changing the rates of MTS (methyltrichlorosilane) pyrolysis and other interior reactions, leading to the lower deposition rate. As the deposition advances, the substrate surfaces are covered by SiC gradually, reducing the growth resistance, and speeding the deposition up to maximum. Meanwhile, the larger the Ar flow, the thinner the MTS in the reactor, and the longer the time for transforming heterogeneous growth into isogeneous growth. In addition, the large Ar flow slows down the increase of HCl density and then the reduction in deposition rate.

Effect of Process Parameters on Deposition

Figure 5 predicts the relationship between MTS density and coating thickness under various Ar flows. It is evident that the coating thins away as the MTS densities. However, it must be mentioned that the effect of MTS density on coating thickness turns into less notable when the Ar flow is larger than or equal to 500ml/min. The decomposition of MTS demands the excess H_2 , nevertheless, the surplus Ar reduces the H_2 density. Therefore, the decomposition of

MTS into SiC is inhibited in some extent. Moreover, accompanying with the increase of MTS density, the process and direction of MTS decomposition alter, resulting in large amount of SiC powders and other gaseous products, and thinning out the SiC coating on C/C surfaces consequently. Figure 6 illustrates the effect of MTS density on coating thickness at the 400ml/min Ar flow, which is derived from the practical tests. Compare Fig.6 with Fig.5, it can be said that the prediction is accordant to the experimental results, indicating the reliability of the model completely. Furthermore, the neural network model is capable to offer more detailed and specific estimation to the deposition with various flows and directly describe the interaction between each procedure factor, proving itself a reasonable and efficient way to simulate the SiC-CVD process.

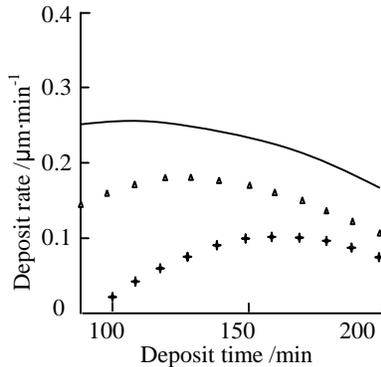


Fig.4 The time effect on deposit rate with different Ar flow
 - 300ml/min; \blacktriangle 400 ml/min; \blackplus 500ml/min

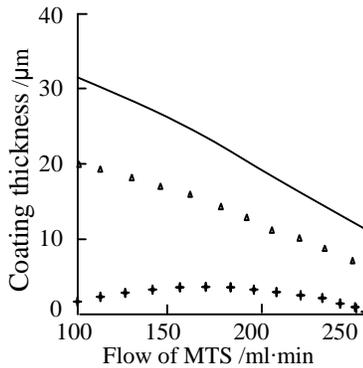


Fig. 5 Effect of MTS on coating thickness under differed Ar flow
 - 300ml/min; 400 ml/min; 500ml/min

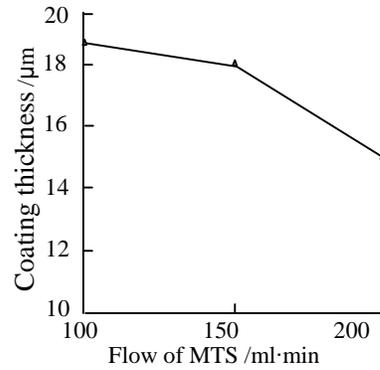


Fig.6 Effect of MTS on coating thickness

Conclusions

- (1) In this paper, the artificial neural network identification theory is applied to research the SiC-CVD process systematically, and the model founded has the capability to estimate the deposition with unknown process parameters. The model estimation agrees with the practical test consequences, proving the reliability of the model. Furthermore, the model reflects the deposition mechanisms and the interaction more thoroughly.
- (2) Combining the orthogonal design with the neural network to plan the learning samples, the demand that the samples distribute on a whole is satisfied, which is required in the neural network modeling of practical complicated procedures. Hence, the amount of work to attain the learning samples reduces, and the model reliability is ensured.
- (3) The method is developed to analyze and determine the interaction between various process factors by the neural network model, providing a new access to judge the interaction existence in the complicated process with multi- influencing elements.

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