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Prediction Model for Studying the Growth Kinetics of Fe_2B Boride Layers during Boronizing

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ABSTRACT

The simulation and modelling of the boriding process are considered as a necessary tool to select the suitable parameters for obtaining an adequate boride layer thickness. In spite of the importance of the boriding process in the industrial field, there are no fully successful mathematical models for simulating the boriding process. In this study, we developed a model based on the application of the artificial neural network (ANN) for the thermochemical boronizing process of the AISI 316L stainless steel. We are attempting to apply the ANN approach to determine the layer's thickness and predict the influence of different parameters on the growth kinetic of the boride layers.
In order to validate the ANN approach, we used experimental data obtained on AISI 316L steel, borided in a liquid medium (70 % borax + 30 % SiC).
The comparison of results obtained by artificial neural network (ANN) model with those given by the mathematical model based on Fick's law and experimental data allow us to validate the ANN model. In addition, the average error generated from the neural network was between 1 and 1.25 µm.

1. INTRODUCTION

Boriding is a thermochemical treatment of steels that permits to have a very resistant layer against corrosion and wear [1]. This phenomenon, based on the diffusion of boron atoms in the iron matrix, generally depends on the nature of the boron source used [1-2]. The boriding medium can be solid (powder or paste), liquid or gas. It is carried out at higher temperatures, generally from 750 to 1050 °C. According to the iron-boron equilibrium diagram [2], the diffusion of boron atoms in the crystal lattice of iron leads to the formation of two kinds of iron boride (FeB and Fe_2B) [3]. The thickness and the quality of the borided layer in a liquid medium treatment depend on the chemical composition of the medium in contact with the surface, on the temperature and on the treatment duration [4].

It is difficult to measure experimentally the thickness of the borided layer [5] due to the saw-tooth morphology of boride layer [6]. In the literature data, the borided layer thickness has been calculated by taking the average distance of every column from the surface [2]. The degree and the teeth length can be reduced by increasing the alloy content [2-7].

Despite the importance of the boriding process in the industrial field, there is no well-detailed model about the growth kinetics of borided layer. Several studies have been undertaken for the boriding process in solid medium [8-9]. For the powders technique, the model of Brakman et al. [10] explains the specific difference of volume between FeB and Fe_2B phases. The growth kinetics of borided layers was studied by empirical models based on Fick's laws [11-12], this model allowed the characterization of the FeB and Fe_2B phases, and the determination of the diffusivity of boron in iron borides.

In the case of boriding process, we can mention the work of Mebarek et al. [13] where they calculated the borided layer thickness and predicted the boron concentration in each phase in a liquid medium.

A growing range of applications of the boriding process, in which the borided layer should be characterized by better and better properties, requires the use of intelligent control systems.

Other methods such as neural networks, fuzzy logic and genetic algorithm became common for this type of process.

Campos et al. [14] used an artificial neural network model to estimate the thickness of the borided layer as a function of the boron paste thickness. In another work [15], they used the fuzzy logic method to estimate the thickness of the borided layer. Genel et al. [16] used the method of artificial neuron network with the back propagation learning algorithm to predict the hardness of borided layer during the boriding process.

The greatest advantage of artificial neural network over other modelling approaches is the capability to model complex, non-linear processes without assuming the form of relationship between input and output variables. Indeed, neural networks have been successfully applied to the classification and approximation of functions.

There are several artificial neural network architectures used in the literature such as multilayer perceptron (MLP), radial basis function network (RBF) and recurrent neural network (RNN).

In this study, we investigate numerically the thermochemical boriding process of the AISI 316L steel immersed in a salt bath (70% borax + 30% SiC) at temperatures between 850 °C and 1050 °C for 2, 4, 6 and 8 hours.

To validate the model based on the artificial neural network model developed in this work, we used the mathematical taken the reference work [13], which is based on Fick's laws and takes into account some thermodynamic properties of the Fe-B phase diagram. In our case, the phase diagram indicated the presence of two phases Fe_2B and γ-Fe.

2. ARTIFICIAL NEURAL NETWORK SIMULATION MODEL

Neural networks are data processing systems; their structure is inspired from the nervous system structure [17-18]. They are modelling tools by learning, which permit the adjustment of very general nonlinear functions into sets of points describing static or dynamic phenomenon [19].

In this study, we used a multilayer perceptron (MLP) wherein the artificial neuron (Figure 1) receives a number of input variables from neurons belonging to upstream level represented by: $x_1, x_2, ..., x_k$. An W_{ki} weight is associated with each of the inputs and is representative of the connection strength.

The weights W_{ki} used for the connections between different layers have much significance in the work of the artificial neural network, and the characterization of the network.

We calculate the output of each neuron (y_i) in the hidden and output layers as follows. We add a bias (θ_i) or threshold value to the activation of a neuron (we call this result n_i) and use the sigmoid function below to get the output.

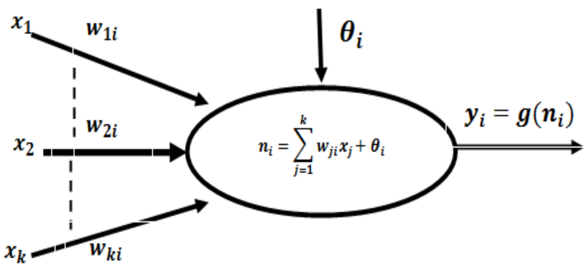

Figure 1. Schematic of an artificial neuron in the MLP network

The artificial neural network used for the boriding process study is composed of three layers, an input layer made up of two neurons (temperature and boriding time), a hidden layer with five neurons and an output layer representing the thickness of borided layer.

The result obtained by the output layer is represented by the following equation:

$$y = g\left(\sum_{j=1}^{5} w_{j1}^{2} g\left(\sum_{k=1}^{2} w_{kj}^{1} x_k + \theta_{j1}^{1}\right) + \theta_{12}^{2}\right) \quad (1)$$

where, θ_{ij}^{k}: represents the bias, w_{ij}^{k}: the weight between neuron i and j, *k* the layer and g: the activation function.

In this type of simulation, we have three important parameters. At Input, we use the treatment time and the boriding temperature. At output, we obtain the thickness of borided layer. The artificial neural network is shown schematically in Figure 2.

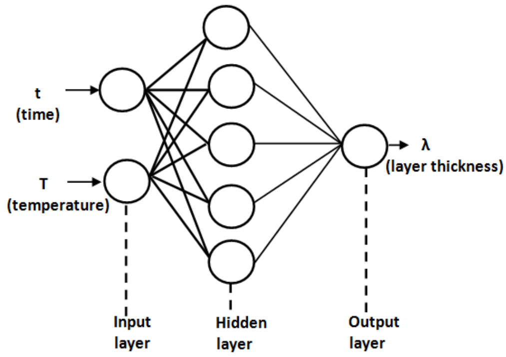

Figure 2. Schematic representation of the artificial neural network for the boronizing simulation process

The activation function used is the sigmoid function given by the following expression:

$$g(n) = 1/(1 + \exp(-n)) \quad (2)$$

The learning algorithm is a mathematical method that modifies the connection weights to converge to a solution that allows the network to perform the desired task. The learning is a parametric identification, which optimizes the weight values of the network [20-21]. During this phase, the behaviour of the network is changed until getting the desired one.

In this study, we use the classical supervised back propagation learning method, which is a learning algorithm suitable for multi-layer neural networks.

Back propagation is the best known learning method, and one of the most efficient for multilayer networks [20].

Learning methods are generally often iterative; they adapt the connection weights after the presentation of each input vector. It is necessary to set the input data many times until the weights converge to stable values.

A training base is the test base, which performs the training of the network and it is used to find a set of optimized weights. The network was trained with the experimental data obtained from the boriding of AISI 316L steel [22].

The weights values (w_{ik}) and values are automatically initialized with a program that we wrote in the C++ language. The number of iterations performed during the training phase is 60000 iterations, during the training phase and the learning rate was set to 0.04.

3. EXPERIMENTAL PROCEDURE

In order to test the validity of mathematical model, we used the results of the boriding experiments on AISI 316L steel taken from our own experimental data recently published in [22]. In that experiment, the samples of AISI 316L stainless steel were selected for boriding treatment.

The chemical composition of AISI 316 L steel (in mass %) is the following: 0.03 % C, 1.3 % Mn, 12.2 % Ni, 0.35% Co,17.4 % Cr,2.28 % Mo,0.44 % Ti, 0.45 % Si and 0.07 % V.

The boriding process were achieved in molten salts, constituted of sodium tetraborate $Na_2B_4O_7$ (70 % in mass) and a reducing agent silicon carbide SiC (30 % in mass).

The use of the silicon carbide (SiC) as a reducing agent led to a single-phase layer (Fe_2B). The thermochemical treatment was done at the three different temperatures 850 °C, 950 °C and 1000 °C with three treatment times 2, 4, 6 and 8 hours.

After the boriding treatments, some samples were sectioned longitudinally to obtain two sections for optical microscopy observation.

4. RESULTS AND DISCUSSION

In the first section, we presented the relative results for the first model of artificial neural network, which we compared to the experimental results [22]. In the second section, we presented the simulation with mathematical model based on Fick's second law [13] and the comparison of the results obtained by these two models.

4.1 Artificial neural network approach

The learning of artificial network was made via the same experimental results [22] used in the first model with 60000 iterations. The convergence rate value of the network is 10^{-6}. To apply the learning algorithm of the network we normalized the experimental data with the following parabolic equation:

$$\lambda = k\sqrt{t} \tag{3}$$

With λ: Fe_2B layer thickness, k: the kinetic constant and t: boriding time.

The learning algorithm purpose is to provide a method to the network, so it can adjust its settings for examples' treatment.

Learning is the process of adapting the parameters of a system to give a desired response to any input or to any stimulation. In Table 1, we gathered the values of borided layer thicknesses obtained by the method of artificial neural networks and their comparison with the experimental results.

Table 1. Comparison between the experimental values and those obtained during the training of the neural network at temperatures of (950 and 1000 °C)

Times (h)	Fe₂B layer thickness Experimental values (µm)			Values obtained by the neural network(µm)		
	2h	4h	6h	2h	4h	6h
950 °C	6	12	18	8.99	13.27	15.45
1000 °C	9	17	24	12.94	19.07	21.73

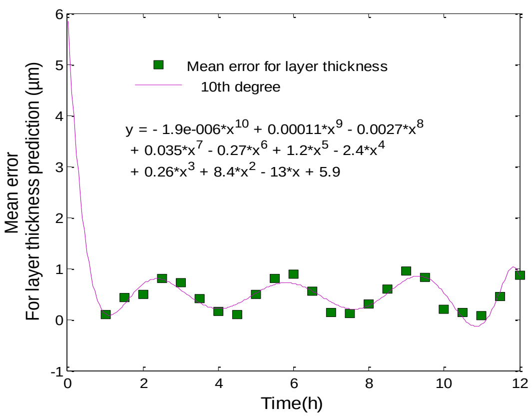

Figure 3. Average error on the Fe_2B layer thickness

We found a good agreement between the experimental data and the data obtained with the neural network at different temperatures.

The mean prediction error of the thickness of borided layer related to different treatments from 850 °C to 1000 °C as a function of time is plotted on Figure 3. We observed that the error shifts between 1 and 1.5 µm for different processing times.

4.2 Mathematical model

The mathematical model used is derived from a previous work by Mebarek et al. [13]. This model is based on the solution of Fick's diffusion equation in a semi-infinite medium on one hand, and on the assumption that the boriding process is an equilibrium process on the other hand. The local thermodynamic equilibrium is quickly reached at each point in the material, from which we can estimate the growth rate at the interface (Fe_2B/γ-Fe) and determine the boride layer thickness. The important parameters for the simulation are the temperature, process time, the diffusivity of boron in each phase and the concentration of boron at the material surface.

For the Fe_2B phase, we calculated the diffusion coefficient with the method given by Bektes et al. [23]. The relation between the boride layer thickness and the boriding temperature is given by:

$$d^2 = D_0.t.\exp({}^{-Q}/_{RT}) \tag{4}$$

where, d is the experimental boride layer thickness (µm), D_0 is the boron diffusion coefficient (µm²/s), t is the boriding time (s), Q is the -activation energy for boron diffusion (J/mol), R is the universal gas constant R=8.314 J/mol K, and T is the boriding temperature (K).

Equation 4 can be written as follows:

$$2.Ln\,(d) = {}^{-Q}/_{RT} + Ln(D_0.t) \tag{5}$$

We can determine the diffusion coefficient after fitting the logarithmic values of the average thickness of boride layer as a function of inverse temperatures.

Consequently, the activation energy for boron diffusion in the Fe_2B layer is determined by the slope obtained from the plot Ln(d) versus 1/T. By Assuming the Arrhenius relation for the diffusion process, one gets Equation (6):

$$D_{Fe_2B} = 6.94\times10^{-5}\exp(-\frac{174.6\times10^3}{RT}) \quad (m^2s^{-1}) \tag{6}$$

where the estimated value of activation energy for boron diffusion is equal to 174600 J/mol.

While for the γ-Fe phase, we kept the same formula as in [6-24]. At the interfaces, we used the results given by Hallemans et al. and Brakman et al. [25-10]. For boron concentrations at the (*Fe_2B/γ-Fe*) interface, we used the following values:

Fe_2B/γ-Fe Interface: $C_B^{Fe_2B/\gamma-Fe} = 8.83\ (wt.\%)$

γ-Fe/Fe_2B Interface $C_B^{\gamma-Fe/Fe_2B} = 35\times10^{-4}\ (wt.\%)$

For boron concentration at the surface 8.854 wt.%, we get the values of the growth rate constants simulated for different temperatures (Figure 4).

The change in the growth rate constant at the Fe_2B/γ-F interface is shown in Figure 4; we note that the growth kinetics of the borided layer depends on the boron concentration and on the process temperature. If the temperature increases, the diffusion rate of boron atoms becomes very fast. The growth kinetics of Fe_2B layers increases according to a parabolic boriding time law; hence, the boron diffusion controls the growth of Fe_2B.

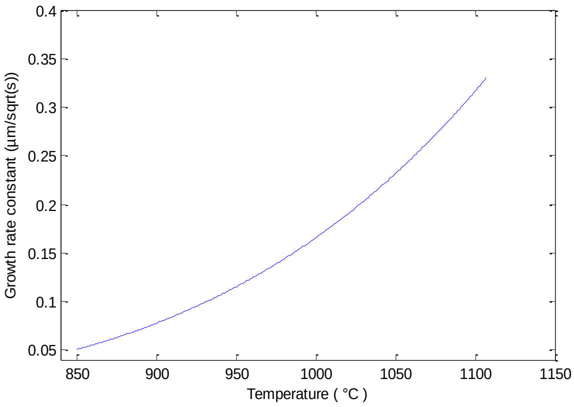

Figure 4. Evolution of the absolute growth rate constant values in function of temperature

From the growth rate constants determined previously, we calculated the thickness of borided layer. The thickness is estimated by assuming that the Fe_2B layer forms instantly at t=0 and covers the surface immediately.

The comparison of the thickness of calculated borided layer with the experimental results is shown in Figure 5. We note that there is a good concordance between the two results (simulation and experiment).

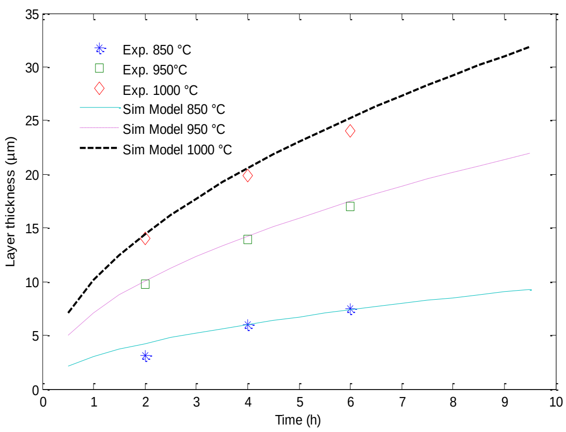

Figure 5. Comparison between the simulated and the measured thickness for various temperatures

The comparison of simulation results with the model based on Fick's second law [13] and with the artificial neural networks' results (ANN) are shown in Figure 6. We note that the results obtained by the artificial neural networks (ANN) are consistent with data from the second Fick's law.

The ANN approach can be used to determine optimal conditions for the process control.

From the achieved results, the methodology of neural network has become an alternative to modelling the boriding process.

In this study, the mathematical model is based on the second Fick's law, we used several parameters and the validity interval of this model is limited to temperatures between 850 °C and 1050 °C.

However, for the artificial neural network model, we used only temperature, time and the learning base.

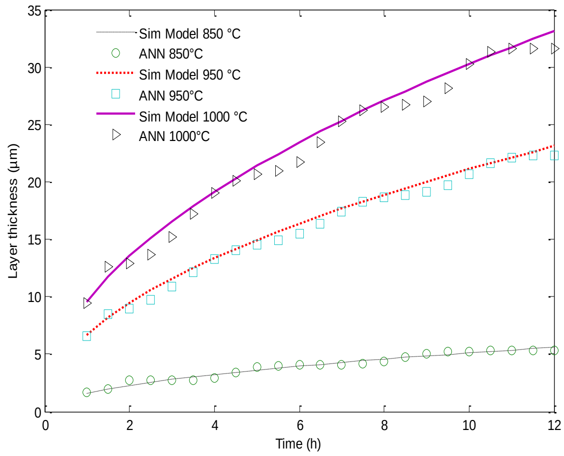

Figure 6. Evolution of the thickness of the boronized layer in function of time

5. CONCLUSIONS

Through this work, it is seen that it is possible to develop artificial neural network model to treat the boriding process. The simulation of the boriding kinetics by this approach gives good results. The comparison of experimental results with our theoretical calculations allows us to confirm the validity of the used approach.

The results of neural network method applied for predicting the borided layer thickness are very satisfying, and they encourage further investigations. The accuracy of prediction depends on the accuracy of measured data, and they should reflect real relations between times, temperature and layer thickness.

With these numerical approaches, one can determine the influence of the different involved parameters, such as the temperature, the boron concentration and the duration of boriding process. The results obtained in this work clearly showed the influence of these parameters.

The main advantage of this technique is the ability of the neural network self-learning. Depending on the process parameters, this network is able to self-adjust by changing the neuron weights until results reach the desired error. Through comparing the results obtained by the artificial neural network to the experimental data, the average error generated from the neural network was between 1µm and 1.25 µm.

In summary, on one hand, for the mathematical model (second Fick's law) we used several parameters which are: (the time, the temperature, the concentration and the concerned interface, the boron surface concentration and the diffusion coefficient of boron in each phase). The validity interval of th model based on second Fick's law is limited to the temperature range 850- 1050 °C.

On the other hand, for the second model (artificial neural network) we used only the temperature, the time and the learning base.

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