LS-SVM approach for modeling the growthe kinetics of FeB and Fe_2B layers formed on Armco iron

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ABSTRACT. *The present study is based on the Least Squares Support Vector Machines (LS-SVM) approach for simulating the boronizing kinetics of Armco iron. This work adopts the Least Square Support Vector Machine for the growth kinetics of FeB and Fe_2B layers. This approach uses the regression technique with the theory of statistical learning LS-SVM has been used to simulate the thickness of each boride layer (FeB or Fe_2B), the input data of the simulation model are the process temperature and the treatment time. The LS-SVM results are compared to experimental data. The good agreement between the two results confirms the validity of the mathematical model. After the validation, the root mean square error and coefficients of determination are calculated to achieve a good performance and a better accuracy. In this work, the comparison results in a value of root mean square error of 0.14 µm for Fe_2B and 0.16 µm for FeB. Furthermore, an equation has been proposed to estimate the thickness of boronized layer as a function of time and temperature using the present model.*

RÉSUMÉ. *La présente étude se base sur l'approche machine à vecteurs de support au sens des moindres carrées (MVS-MC) pour simuler la cinétique de boruration du fer Armco. Ce travail adopte la machine à vecteurs de support au sens des moindres carrées pour la cinétique de croissance des couches FeB et Fe_2B. Cette approche utilise la technique de régression avec la théorie de l'apprentissage statistique. Elle a été utilisée pour simuler l'épaisseur de chaque couche (FeB ou Fe_2B) et les données à entrer dans le modèle de simulation sont la température du procédé et la durée du traitement. Les résultats de l'approche (MVS-MC) ont été comparés aux données expérimentales. Le bon accord entre les deux résultats confirme la validité du modèle mathématique. Après validation, l'erreur quadratique moyenne et le coefficient de détermination ont été calculés pour parvenir à une bonne performance et meilleure précision. La comparaison des résultats a donné les valeurs de l'erreur quadratique moyenne égales à 0.14 µm pour Fe_2B et 0.16 µm pour FeB. De plus, une équation a été proposée pour estimer*

l'épaisseur de la couche borurée en fonction du temps et de la température en utilisant le présent modèle.

KEYWORDS: *LS-SVM, prediction, boronizing, model, simulation.*

MOTS-CLÉS: *MVS-MC, prédiction, boruration, modèle, simulation.*

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1. Introduction

Boronizing is a thermochemical surface treatment for hardening the metallic surfaces. It allows obtaining highly resistant layers to corrosion and produces a hard, wear resistant boride layer. The hardness of the treated surface can attain about 2000 Hv (Allaoui *et al.*, 2006). This treatment is applied to ferrous materials, but also to some nonferrous materials (Keddam *et al.*, 2010). The boronizing is carried out between 850°C and 1050°C for 0.5 to 12h (Mebarek *et al.*, 2012). In this process, active boron atoms diffuse into the surface of substrate metal or alloy in order to produce a layer of borides (Campos *et al.*, 2003).

The source of boronizing can be solid, liquid or gaseous (Matuschka, 1980). The boronizing process depends generally on the nature of the source that provides the boron (Mebarek *et al.*, 2015). The boronizing is based on the diffusion of the boron atoms on the iron's matrix, with the possibility of chemical reactivity to give borides (Ueda *et al.*, 2000).

According to the Fe-B equilibrium phase diagram, the dispersion of boron in the crystal lattice of iron results in the formation of two kinds of iron borides (FeB and/or Fe_2B) (Kubaschewski,1982). The formation of the Fe_2B and/or FeB layer depends on the activity and the chemical concentration of boron (Jain & Sundararajan, 2002). For a low boron potential, only the formation of Fe_2B phase occurs. In the case of a higher boron activity, we notice the existence of two phases: FeB and Fe_2B. The quality and the thickness of boronized layer depend on the boronizing techniques employed (Ozbek & Bindal, 2011), the chemical composition of the boron source, the temperature and the treatment duration (Mebarek *et al.*, 2016; Keddam, 2004).

Mathematical models have been used by several authors for studying the growth kinetics of boride layers duration. One of those mathematical approaches has been developed by Campos *et al.* (Campos *et al.*, 2010) to study the boronizing process. Their model requires the knowledge of the influence of different parameters: temperature, time, and boron concentration. It is based on Fick's second law, and the mass balance equations of Fe_2B and FeB phases. However, they rely on experimental data, and they are highly sensitive to the measurement of the boride layer thicknesses. In practice; it is very hard to experimentally measure the thickness of the boride layer (Bouaziz *et al.*, 2009).

To deal with the error caused by the experimental measurements, a variety of prediction models have been suggested in the literature (Ozdemir *et al.*, 2009; Campos *et al.*, 2007), for example, Campos *et al.* have used an artificial neural network model (ANN) to evaluate the thickness of borided layer according to the thickness of boron

paste; while other authors have employed a fuzzy logic (FL) method for the same objective.

To predict the hardness of boronized layer consisting of FeB and Fe_2B during the boronizing process, Genel *et al.* (Genel *et al.*, 2002) have used the method of artificial neural networks.

Recently, the SVMs approach (Support Vector Machines) has been gaining more and more attention thanks to its ability to solve a large number of classification and regression problems. This approach takes advantage of the algorithms already developed in the machine learning community (Vapnik., 2005). Training an SVM involves solving a constrained quadratic optimization problem (Wang *et al.*, 2005). They are not affected by the problem of local minima because their training is equivalent to a convex optimization.

The LS-SVM (Least-Square Support Vector Machine), proposed by Suykens and Vandewalle (Suykens *et al.*, 2001), is a simplification of the SVM approach. The LS-SVM has the same advantages as the SVM, in addition to the fact that it requires solving only a set of linear equations, which is much easier and computationally simpler.

The flexibility of this approach is due to the use of kernel functions (Mishra *et al.*, 2014, Tian *et al.*, 2017). It is a more powerful alternative to parametric methods.

The hyper-parameters of SVMs approach (kernel function and regularization parameter) are very influencing on the LS-SVM performance (David and Sánchez, 2003).

In this paper, a LS-SVM regression model is proposed to estimate the boronizing kinetics of Armco iron by determining the boride layer thickness. The main objective of this study is to predict the influence of the process temperature and the treatment time on the kinetics of formation of Fe_2B and FeB layers at the surface of Armco iron based on the literature data.

2. LS-SVM model

This section of the paper presents the principle description of the LS-SVM method. More details on the LS-SVM method can be found in references (Steinwart & Christmann, 2008; Anandhi *et al.*, 2008).

The present LS-SVM model is an alternate formulation of SVM regression proposed in (Tripathi *et al.*, 2006).

Consider a given training set of N data points $\{(x_i, y_i), i = 1, \mathrm{K}, N\}$

Where x_i is the "i-th" input data (x= $[x_i, \mathrm{K}, x_n] \in R^n$) the x_i constitutes the input of the model, and $y_i \in R$ is the value of the desired output.

The input data used for our LS-SVM model are t (time) and T (temperature), x = [t, T], and the output is the thickness of boride layer λ , y = [λ].

In feature space LS-SVM models take the form:

$$y(x) = \sum_{j=1}^{h} w_j \varphi_j(x) + b = w^T \varphi(x) + b \quad (1)$$

Where:

φ(x): Non-linear mapping function.

w : is the weight vector, $w \in \mathrm{R^N}$,

and: is the bias term , $b \in \mathrm{r}$;

The goal of the support vector machine training is to find the particular hyperplane that minimize the training error (Suykens *et al.*, 2002).

The training phase involves estimating the appropriate values of the set of parameters w. These parameters are estimated and adjusted by minimizing the cost function $\psi_L(w,\mathrm{e})$, this problem of optimization can be represented as follows:

Minimize:

$$\psi_L(w,\mathrm{e}) = \frac{1}{2}\mathrm{w^T w} + \frac{1}{2}\gamma \sum_{\mathrm{i=1}}^{\mathrm{N}} \mathrm{e_k^2} \quad (2)$$

$$y_i - \hat{y}_i = e_i \quad , \mathrm{i=1,..N}$$

Subject to: $$\mathrm{y(x) = w^T \varphi(x_i) + b + e_i \, , i = 1, \dots , N} \quad (3)$$

Where

e_i = error variable.

γ : is a regularization parameter, and $\hat{y}_i$ is the actual model output.

The first term of the cost function (eq.2), representing the weight decay, is responsible of finding a smooth solution, which is used to regularize the weight sizes and penalize the large weights.

The second term of the cost function, representing the penalty function, is the regression error for all training data.

The following equation for layer thickness (λ) prediction has been obtained by solving the above optimization problem.

With the restriction of equation (3), the solution of the optimization problem can be obtained from the Lagrangian function as:

$$L(w,b,e,\alpha) = \frac{1}{2}||w||^2 + \frac{1}{2}\gamma \sum_{i=1}^{N} e_i^2 - \sum_{i=1}^{N} \alpha_i \{w^T \varphi(x_i) + b + e_i - y_i\} \quad (4)$$

Where α_i, $\mathrm{i = 1 \dots N}$ are the Lagrange multipliers, and b is the bias term.

The following equations represent the optimality condition:

$$\begin{cases} \frac{\partial L}{\partial W} = 0 \rightarrow \ \ w = \sum_{k=1}^{N} \alpha_k \varphi(x_k) \\ \frac{\partial L}{\partial b} = 0 \rightarrow \ \sum_{k=1}^{N} \alpha_k = 0 \\ \frac{\partial L}{\partial e_k} = 0 \rightarrow \ \ \alpha_k = \gamma e_k \ \ , k = 1 \ldots N \\ \frac{\partial L}{\partial \alpha_k} = 0 \rightarrow \ \ w^T \varphi(x_k) + b + e_k - y_k = 0 \ , k = 1 \ldots N \end{cases} \tag{5}$$

Then:

$$w = \ \sum_{i=1}^{N} \alpha_i \varphi(x_i) = \ \sum_{i=1}^{N} \gamma e_i \varphi(x_i) \tag{6}$$

Where a positive definite Kernel is used as follows:

$$K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j) \tag{7}$$

An important result of this approach is that the weights (w) can be written as linear combinations of the Lagrange multipliers method with the corresponding training data (x_i).

By substitution of (6) into (1), the following result is obtained:

$$y = \sum_{i=1}^{N} \alpha_i \varphi(x_i)^T \varphi(x\,) + b \tag{8}$$

For a given point, yi can be evaluated by:

$$y_i = \sum_{i=1}^{N} \alpha_i \varphi(x_i)^T \varphi(x_j\,) + b \tag{9}$$

The above conditions of optimality can be expressed as the solution to the following set of linear equations after eliminating w and ei.

$$\begin{bmatrix} K + \frac{1}{\gamma} & 1_N \\ 1_N^T & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ b \end{bmatrix} = \begin{bmatrix} y \\ 0 \end{bmatrix} \tag{10}$$

Where K denotes the kernel matrix with i,jth element given by equation (7). $1_N = [1, .. 1]^T$, Hence, the solution is given by:

$$\begin{bmatrix} \alpha \\ b \end{bmatrix} = \begin{bmatrix} y \\ 0 \end{bmatrix} \begin{bmatrix} K + \frac{1}{\gamma} & 1_N \\ 1_N^T & 0 \end{bmatrix}^{-1} \tag{11}$$

$K(x_i, x_j) = \varphi^T(x_i)\varphi\,(x_j)$ is the kernel function, from the estimation function, we represent the model as the following equation:

$$y(x) = \sum_{i=1}^{N} \alpha_i K(x_i, x) + b$$

For a point x_j to be evaluated it is:

$$y_j(x) = \sum_{i=1}^{N} \alpha_i K(x_i, x_j) + b \quad (12)$$

In our LS-SVM model case-study, the radial basis function (RBF) kernel is chosen to map the input data. The RBF function is selected thanks to its simplicity and accuracy. It is given by:

$$K(x, x_i) = exp\left\{-\frac{\|x-x_i\|^2}{\sigma^2}\right\}, k=1,...,N$$

Where, σ is a constant representing the "width" of this Gaussian. It can be adjusted to control the expressivity of RBF. The x_i determines the centre of this function. The choice of a kernel function depends on the problem at hand; it depends on what we are trying to model. There are several choices of kernel functions: linear, polynomial, sigmoid, splines or radial basis function (RBF).

It is worth mentioning that accuracy of LS-SVM model with RBF kernel is related to the choice of parameters (the width σ of the RBF kernel and the parameter γ).
The result (y) is the weighted sum of the values of the $K(x, x_i)$ kernels, where the weights are the calculated α_k Lagrange multipliers.
The above LS-SVM has been adopted to determine the boronizing kinetics of Armco iron in case of a bilayer configuration (FeB and Fe_2B).

3. The collection of the data

The data used for the training and the testing of the method were collected from the literature (Brakman *et al.*, 1989). An application to calculate the boronized layer thickness based on the mathematical model of (Keddam & Chentouf, 2005) is also used. The data have been divided into two sub-sets; a training dataset to construct the model, and a testing dataset to estimate the model performance.

3.1. Experimental data

The validation of the simulation in this study is based on the Brakman *et al.* experimental data. Brakman et al used the technique of powder-pack boronizing for treating the Armco iron substrate.

The chemical composition of Armco iron to be pack-borided is given in Table 1.

Table 1. Chemical composition of Armco iron samples

Elements	Fe	C	Mn	Ni
%(wt)	Balance	0.005	0.0013	0.004

Boronizing in powders is advantageous because of its simplicity and cost-effectiveness in comparison to the other processes.

The selected temperature interval is from 850 to 1050°C, and that of the treatment time is between 0.5 and 10 h.

The bilayer configuration FeB and Fe2B was observed after the boronizing. The experimentally determined thickness of each boride layer (FeB or Fe2B) was averaged from 20 measurements made in different points on the cross-sections of treated samples.

4. Results and discussions

In this part, the proposed approach with Radial Basis Function (RBF) kernel is implemented in (Scilab environment version 6.0) and tested on selected datasets. In the simulation we assume that the experimental data of Fe_2B growth layer follows the relationship $y = k.t^{½}$ (where t is boronizing time (s), and k is the growth rate constant). As mentioned earlier, this study uses radial basis function as a kernel function. So in order to get a good optimization of results, we are proceeding by varying the two parameters: γ and σ during the training of LS-SVM.

Figure 1 shows the variation of Fe_2B boride layer thickness calculated by simulation (LS-SVM methods) as a function of the process temperature and the treatment time. We notice that the simulation results are in a good agreement with the experimental measurements.

Using the numerical model, the thickness of the Fe_2B layer and the rate kinetic constant can be easily estimated.

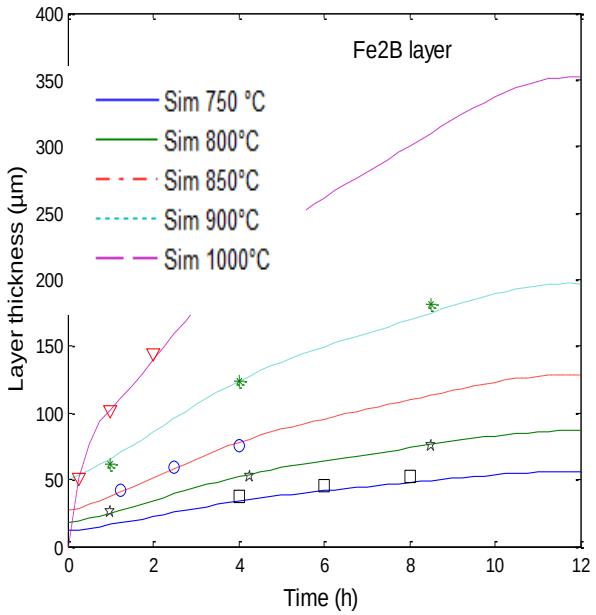

Figure 1. Comparison between the experimental data and the estimated values of the Fe_2B layer thickness. The symbols denote the experimental values

Figure 2 shows the variation of FeB boride layer thickness calculated according to the same parameters: the temperature and the treatment time. We can also notice the good agreement between the simulation and the experimental data. This allows us to confirm the validity of the LS-SVM approach.

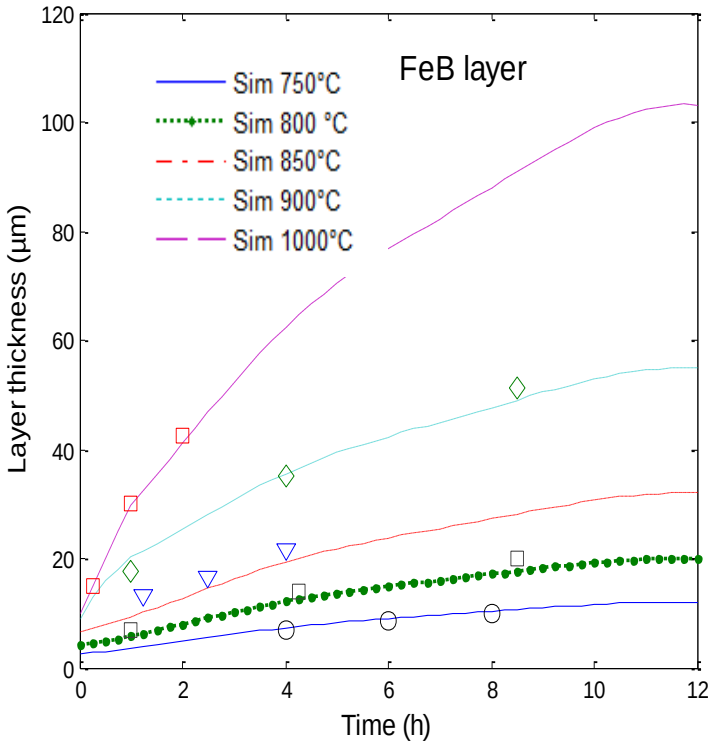

Figure 2. Comparison between the experimental data and the estimated values of the FeB layer thickness. The symbols represent the experimental values

From figures 1 and 2, we note that the LS-SVM approach can be used to determine the optimal conditions to control the process. From the obtained results, we can say that the LS-SVM approach can be considered as a very powerful alternative to modelling the boronizing process. For example, compared to the mathematical model based on Fick's law that uses several parameters (temperature, time and boron concentration), the LS-SVM approach uses only the learning base. This presents a limitation for the validity interval of the mathematical model based on Fick's law.

The validity and accuracy of LS-SVM approach is checked, by calculating the average error made during the calculation of the thickness of each boride layer (FeB or Fe_2B) for different temperatures and treatment durations.

The mean error made in the calculation of the thickness of boronized layer for different treatments temperature is plotted on figure 3. While the prediction error of the Fe_2B layer thickness is limited between 1 and 3.75 µm, that of the FeB layer varies in an even narrower interval: between 0.4 and 1.35 µm. That is the case for all the considered processing temperatures.

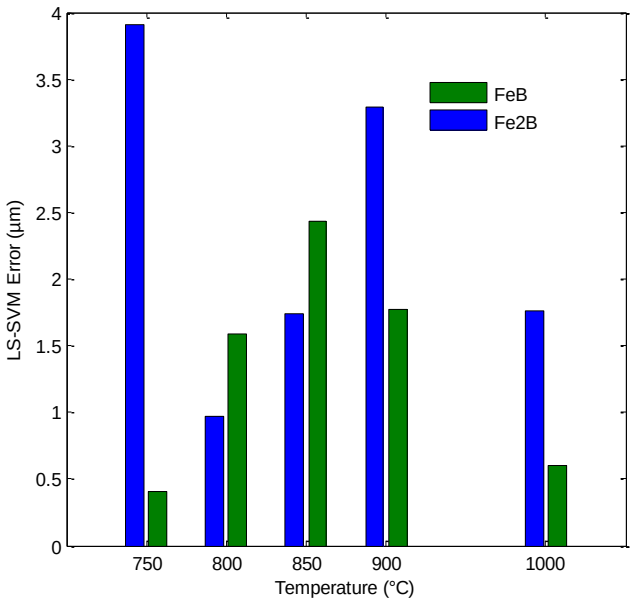

Figure 3. The error between the experimental data and the estimated values

To analyze further the validity and the performance of LS-SVM model, a comparison between the predicted results and the experimental values was performed based on two statistical parameters.

The root mean square error (RMSE) and coefficient of determination R^2 are calculated using the following equations:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(X_{i\ exp} - X_{i\ pred})^2} \tag{13}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(X_{i\ exp} - X_{i\ pred})^2}{\sum_{i=1}^{n}(X_{i\ pred} - \overline{X})^2} \tag{14}$$

Where

n: is the number of the data samples

X_{iexp} and X_{ipred} are the experimental value (desired) and the predicted value.

$\overline{X}$: is the mean of the experimental data values.

Table 2. The performance evaluation of the LS-SVM approach (for T=1000°C)

Phase	Fe2B	FeB
Root mean square error (RMSE)	0.141	0.160
Coefficient of determination (R^2)	0.993	0.992

From table 2, the results show that the LS-SVM is very powerful in predicting the boronized layer thickness. The proposed approach has a good root mean square error (RMSE) and R^2 value.

The interpolation equations of the LS-SVM model results for each temperature are shown in Table 3. The validity domain of each interpolation equation listed in Table 3 is between 1 and 12 h of treatment time at a given boriding temperature.

Table 3. Interpolation equations of the boronized layer thickness calculated with the LS-SVM model

Temperature °C	Thickness interpolation of boride layer λ(t) en µm
850	$\lambda_{FeB} = 27 \times 10^{-5}t^4 + 0.0044t^3 + 0.12t^2 + 3.8t + 5.9$ $\lambda_{Fe_2B} = 0.0011t^4 - 0.018t^3 - 0.47t^2 + 15t + 24$
900	$\lambda_{FeB} = -0.0042t^4 + 0.12t^3 - 1.4t^2 + 10t + 10$ $\lambda_{Fe_2B} = 0.0016t^4 - 0.026t^3 - 0.68t^2 + 22t + 46$
1000	$\lambda_{FeB} = -0.0072t^4 + 0.21t^3 - 2.5t^2 + 20t + 11$ $\lambda_{Fe_2B} = -0.039t^4 + 1.1t^3 - 12t^2 + 79t + 26$

5. Conclusions

In this paper, the least squares support vector machine was applied to predict the growth kinetics of FeB and Fe_2B layers formed at the surface of Armco iron. It was also used to estimate of each boride layer thickness (Fe_2B or FeB) for the given boriding conditions.
The main advantage of this technique was the ability of LS-SVM method for self-learning. The training of LS-SVM method was based on data from the literature.

The good agreement between the predictions of the proposed approach and the experimental results confirmed the validity of the LS-SVM model. In fact, the comparison results in n root mean square error of 0.14 µm for the Fe_2B phase and 0.16 µm for the FeB phase.

This study showed that the developed LS-SVM approach could be considered as a robust tool for the determination and the prediction of boronizing kinetics of Armco iron.

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